Digital Radiography by Laser Scanned Readout of Amorphous Selenium

by

David MacKenzie Hunter

A thesis submitted in conformity with the requirements for the Degree of Masters of Science

Department of Medical Biophysics

University of Toronto

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Abstract

A theoretical model is presented of a method to acquire digital radiographs using photoconductively activated switches (PASs) formed at the interface of amorphous selenium (a photoconductor) and glass. It is shown that the method would be suitable for both radiography and fluoroscopy if the assumption is made that the bulk photoconductive properties of amorphous selenium hold at the interface. In order to test this assumption experimental measurements of lateral photoconductivity at an amorphous-selenium (a-Se) glass interface were performed with 442 nm laser pulses ranging from 1 µs to several ms duration. It was found that surface photoconductivity is weaker and shorter lived than that in a-Se bulk time of flight (BTOF) measurements. The surface photoconductivity can be explained by supposing that the electrons and holes thermally diffuse to the surface where they are trapped. A theory of surface photoconductivity is developed and numerically solved, giving general agreement with experiment.
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- Everyone in John's group;
- Norm and Gord from the Yaffe camp;
- All my living friends and those many friends and acquaintances who have died from AIDS.
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<td>AC</td>
<td>alternating current</td>
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<tr>
<td>AOM</td>
<td>acousto optic modulator</td>
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<td>a-Se</td>
<td>amorphous selenium</td>
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<td>a-Si:H</td>
<td>hydrogenated amorphous silicon</td>
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<td>BTOF</td>
<td>bulk time of flight</td>
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<tr>
<td>CCD</td>
<td>charge coupled device</td>
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<tr>
<td>CdSe</td>
<td>cadmium selenide</td>
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<td>CN</td>
<td>Crank Nicolson</td>
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<td>c-Si</td>
<td>crystalline silicon</td>
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<tr>
<td>CSIM</td>
<td>charge simulation method</td>
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<tr>
<td>CT</td>
<td>computed tomography</td>
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<tr>
<td>CW</td>
<td>continuous wave</td>
</tr>
<tr>
<td>DC</td>
<td>direct current</td>
</tr>
<tr>
<td>DCE</td>
<td>differential charge-collection efficiency</td>
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<tr>
<td>DQE</td>
<td>detective quantum efficiency</td>
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<tr>
<td>ehp</td>
<td>electron hole pair</td>
</tr>
<tr>
<td>eV</td>
<td>electron Volt</td>
</tr>
<tr>
<td>FET</td>
<td>field effect transistor</td>
</tr>
<tr>
<td>FTCS</td>
<td>forward time centred space</td>
</tr>
<tr>
<td>ITO</td>
<td>indium tin oxide</td>
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<tr>
<td>kTC</td>
<td>&quot;thermal noise&quot;</td>
</tr>
<tr>
<td>kVp</td>
<td>peak kilo-Voltage (x-ray tube)</td>
</tr>
<tr>
<td>lp/mm</td>
<td>line pairs per millimetre</td>
</tr>
<tr>
<td>LU</td>
<td>lower and upper (triangles of matrix)</td>
</tr>
<tr>
<td>μR</td>
<td>micro Roentgen</td>
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<tr>
<td>mR</td>
<td>milli Roentgen</td>
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<tr>
<td>MR</td>
<td>magnetic resonance</td>
</tr>
<tr>
<td>MTF</td>
<td>modulation transfer function</td>
</tr>
<tr>
<td>NPIXDP</td>
<td>non-pixellated dual photoconductor readout</td>
</tr>
<tr>
<td>PAS</td>
<td>photoconductively activated switch</td>
</tr>
<tr>
<td>PC</td>
<td>personal computer</td>
</tr>
<tr>
<td>PID</td>
<td>photoinduced discharge</td>
</tr>
<tr>
<td>PIXDP</td>
<td>pixellated dual photoconductor readout</td>
</tr>
<tr>
<td>PMT</td>
<td>photomultiplier tube</td>
</tr>
<tr>
<td>QE</td>
<td>quantum efficiency</td>
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<tr>
<td>RC</td>
<td>resistance capacitance product</td>
</tr>
<tr>
<td>SiO₂</td>
<td>silicon dioxide</td>
</tr>
<tr>
<td>SNR</td>
<td>signal to noise ratio</td>
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<tr>
<td>STOF</td>
<td>surface time of flight</td>
</tr>
<tr>
<td>TV</td>
<td>television</td>
</tr>
<tr>
<td>3D</td>
<td>three dimensional</td>
</tr>
<tr>
<td>TFT</td>
<td>thin film transistor</td>
</tr>
<tr>
<td>TOF</td>
<td>time of flight</td>
</tr>
<tr>
<td>TTL</td>
<td>transistor transistor logic</td>
</tr>
<tr>
<td>2D</td>
<td>two dimensional</td>
</tr>
<tr>
<td>US</td>
<td>ultrasound</td>
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\( \alpha \): optical attenuation coefficient
\( a \): width of 2D charge strip element in CSIM
\( a' \): constant used in formula to approximate Onsager photogeneration efficiency
\( A \): area
\( B \): boundary vector used in CSIM
\( b \): constant used in formula to approximate Onsager photogeneration efficiency
\( c \): electric field dependent charge collection volume in a PAS pixel element
\( C \): capacitance
\( C_i \): capacitance of PID pixel to the top dielectric electrode
\( C_{se} \): capacitance of PAS pixel electrode to the top and bottom bias electrodes
\( C_{pa} \): capacitance of PAS pixel electrode to the left readout rail
\( C_{pr} \): capacitance of PAS pixel electrode to the right readout rail
\( C_{rd} \): total readout capacitance presented to charge amplifier
\( C_{Se} \): capacitance of PID pixel to the bottom a-Se electrode
\( d_i \): width of PAS pixel
\( d \): width of PAS readout rail
\( d_{se} \): thickness of a-Se layer
\( D \): dose or diffusion coefficient or diameter of laser beam
\( E \): electric field magnitude
\( E_{ag} \): average gap field
\( E_{PAS} \): mean electric field magnitude across PAS readout gap
\( E_{PID} \): electric field magnitude across a-Se Layer of PID plate
\( E_x \): x-ray beam energy
\( \varepsilon \): dielectric constant of material
\( \varepsilon_0 \): permittivity of vacuum
\( \varepsilon_r \): relative dielectric constant of material
\( \varepsilon_{se} \): dielectric constant of a-Se
\( \Phi_{op} \): number of optical quanta used to switch a PAS element
\( \Phi_a \): number of absorbed x-ray quanta in a PAS element
\( \Phi \): potential
\( \Phi_i \): number of x-ray quanta per unit area
\( \Phi_{er} \): reference potential in CSIM modelling
\( f \): # floating electrode segments in CSIM or temporal frequency
\( f' \): # electrode segments on a floating electrode in CSIM
\( F \): fraction of total pixel charge injected into PAS readout gap
\( \gamma \): ratio of electrons to holes
\( g \): gain
\( G \): photogeneration rate
\( G(x,y) \): 2D potential source function for a CSIM charge strip
\( G \): two dimensional source matrix used in CSIM
\( \eta \): photogeneration efficiency
\( h \): Planck's constant
\( i \): dummy index
List of symbols

l: light intensity
j: dummy index or current
J: current
k: Boltzmann's constant
k:\textsuperscript{r}: Rose's criterion
k:\textsuperscript{c}: constant related to the energy required to create a free charge ion pair in a-Se
k: zero input capacitance charge amplifier noise constant
k:\textsuperscript{r}: slope of charge amplifier noise increase with input capacitance
\lambda: line charge density or wavelength of light
l: dummy index
L: potential source function for a CSIM charge line or volume illumination rate
\Lambda: signal coupling efficiency
\Lambda:\textsuperscript{c}: signal coupling efficiency with continuous illumination
\Lambda:\textsuperscript{p}: signal coupling efficiency with pulsed illumination
\mu: mobility
\mu:\textsuperscript{c}: carrier mobility
\mu:\textsuperscript{n}: electron mobility
\mu:\textsuperscript{p}: hole mobility
\mu:\textsuperscript{abs}: x-ray energy absorption coefficient
\mu:\textsuperscript{a}: x-ray attenuation coefficient
\mu:\textsuperscript{en}: x-ray energy attenuation coefficient
m: # floating electrodes in CSIM or dummy index
v: frequency
\xi:\textsuperscript{r}: term in Onsager expansion
\xi:\textsuperscript{c}: term in Onsager expansion
n: # total electrode segments in CSIM or electron density or dummy index
N: number of unknowns in CSIM equation
N:\textsubscript{A}: amplifier readout noise
N:\textsubscript{TR}: thermal readout noise
N:\textsubscript{O}: shot noise
N:\textsubscript{T}: total readout noise
N:\textsubscript{x}: x-ray quantum noise
p: # fixed potential electrode segments in CSIM or hole density
p:\textsubscript{g}: geometric pixel pitch charge collection volume in a PAS pixel element
q: integral quantum unit of electric charge
Q: charge stored on a PAS element
\rho: mass density
r:\textsubscript{g}: initial separation of a geminate electron and hole in Onsager model
r:\textsubscript{ref}: reference position in CSIM model
R: scatter to primary ratio
R:\textsubscript{T}: thermal recombination rate
\sigma: surface charge density or particle cross section
s: # space-charge lines in CSIM
S: signal
S:\textsubscript{r}: surface recombination velocity
\tau: characteristic time
List of symbols

\( \tau_{nd} \): electron detrapping time  
\( \tau_{ph} \): hole detrapping time  
\( \tau_{et} \): electron trapping time  
\( \tau_{pt} \): hole trapping time  
\( t \): time or thickness  
\( T \): absolute temperature  
\( v \): velocity  
\( V \): Voltage  
\( V_f \): floating electrode potentials in CSIM  
\( W_\pm \): energy required to create a free ion pair  
\( x \): Cartesian coordinate  
\( X \): detector x-ray exposure  
\( X \): unknown charge distribution vector in CSIM  
\( x_{\text{chg}} \): total x-ray derived charge on a pixel electrode in CSIM  
\( y \): Cartesian coordinate  
\( y_p \): characteristic penetration depth of light into a-Se layer  
\( z \): Cartesian coordinate  
\( z_{\text{exp}} \): length of illumination line in STOF experiments
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Chapter 1

Introduction
1.0 Introduction

In this chapter an overview of radiological imaging will be given with an eye on methods to achieve a satisfactory digital radiographic method. It will be argued that electrostatic methods based upon the photoconductor amorphous selenium (a-Se) offer some of the best approaches to digital radiography. In particular, photoconductive readout of a-Se has been previously shown to take advantage of the high resolution inherent from a-Se, but suffered from certain problems such as a long readout time. The idea of a new photoconductive surface readout method to overcome this and other problems is introduced as the main body of research in the remainder of the thesis.

1.1 A brief history of radiology

At the time this thesis was written, one hundred years had just elapsed since the discovery of x-rays by Wilhelm Conrad Roentgen. The medical possibilities of x-rays were immediately evident when Roentgen saw the ghostly shadow of the bones of his own hand as he held a small lead disk in front of a barium platinocyanide phosphor screen that glowed when struck by the new "x-rays". Roentgen was mistrustful of his own senses and started using photographic film to record images for objectivity and permanency. It was recognized that x-rays could ionize air and images were also initially created electrostatically by capturing ions on an insulating surface. Later by dusting the surface with red lead and sulphur particles, which would be preferentially attracted to the regions containing charge, the image was made visible. This very early electrostatic imaging method is shown in Fig. 1.1 and note how the electric field lines guide the ions vertically to the collecting surface. However film became the preferred recording medium probably because of its greater sensitivity and better image quality compared to the electrostatic method then available.
Fig. 1.1 X-ray photons have energies much higher than the binding energies of chemical bonds and thus ionize air, water etc. when they undergo an electromagnetic interaction. This fact was used very early on to create electrostatic images as shown here. The vertical electric field between the two electrode plates separates the positive and negative ions and draws them directly to the two electrode surfaces without introducing sideways movement or blurring of the image. However the ionizing property of x-rays introduces a health risk and one goal of radiology is to create high quality images with the smallest amount of radiation possible.

Fig. 1.2: Screen-film radiography. Phosphor screens absorb a large fraction of the incident x-rays (a high QE) and emit a large number of light photons (a high gain) for each absorbed x-ray. The emitted light escapes from the phosphors through a diffusion or random walk process and subsequently is absorbed by the film sandwiched between the screens. Two screens are used to maximize the absorption of x-rays. The diffusion of the light in the screens to the film causes blurring of the image.
It was not fully appreciated in the early years that x-rays could be a danger to health. X-ray tubes were unshielded and physicians made no attempt to protect themselves from x-rays when imaging patients. The glass plate films used to capture the image were very insensitive and exposure times could be as long as an hour (in part since the number of x-rays interacting with an x-ray film, or the quantum efficiency (QE), is typically only about 1%; the rest pass through the film and are wasted) resulting in large radiation doses to the patient. The ill effects of exposure to x-rays were more often skin burns (x-ray dermatitis) but malignancy also occurred and several hundred physicians died before adequate protection measures came into effect.

Practical "intensifying screens" made of calcium tungstate phosphor were developed in 1916 but did not come into widespread use until the 1920s. These remained the principal workhorse of radiography until the 1970s, when faster rare earth screens were introduced. Phosphors dramatically increase sensitivity (~100-1000) compared to direct detection of x-rays by film since they have a QE of about 50% and generate many thousands of light photons (gain) for each absorbed x-ray photon. Phosphor screens have made general radiography possible by reducing exposure times and x-ray tube loading to acceptable levels, even for the thickest body parts and patients. However phosphors degrade image resolution since they must be fairly thick (several 100 microns) and the light generated in the phosphor layer must diffuse to the film in contact with the screen as shown in Fig. 1.2.

1.2 Biological constraints for radiological imaging

Because x-rays are ionizing they create free radicals in the body which can lead to biological damage. It has not been established if there is a safe lower limit of exposure to ionizing radiation. However it should be noted that there is a great deal of variability in natural background radiation levels and these levels are generally greater than those encountered from the medical use of x-
rays. Indeed, it has been suggested by some\textsuperscript{5} that there is even a positive effect of low levels of radiation which might cause an increase in activity of the immune system. Despite these caveats, it is currently assumed for the basis of radiation protection, that radiation exposure should be kept to a minimum. Thus the goal of radiographic imaging is to use the least amount of radiation theoretically possible to form an image of a certain quality.

1.3 Radiological imaging requirements

1.3.1 Diagnostic x-ray energy range

The useful diagnostic energy range of x-rays is from about 18 to 150 keV. At energies below 18 keV too much energy is absorbed (dose) to safely form an image. At energies above 150 keV radiological contrast is greatly diminished. A radiological detector must be capable of absorbing nearly all of the radiation incident upon it, and convert the absorbed energy with sufficient gain, such that the intrinsic noise of the detector is not greater than the signal generated by the x-rays.

1.3.2 Resolution

The low frequency limit of resolution is set by the largest body part to be imaged, typically the chest or abdomen. Diagnostic energy x-rays cannot be easily focused. Therefore the image detector must be capable of being scaled up to a size of about 14"x17". This is a major consideration if one wishes to use solid-state imaging sensors such as CCDs (charge coupled device) which are made of crystalline silicon (c-Si). Such devices are no larger than a few square inches and are also limited to about 1000 pixels along a row due to the very high inter-pixel charge transfer efficiency required.

Ideally the high frequency limit of resolution is set by what is considered an acceptable dose. In mammography, the highest dose and resolution radiographic procedure, resolution of up
to 16 lp/mm is achievable with modern (mammographic) screen-films. However, the modulation transfer function (MTF) at that frequency is very low (1%). The MTF is a measure of how well spatial frequencies are transferred in an imaging system. X-rays are quanta, and apart from detector limitations, the limiting resolution is set by the number of quanta that are present per unit area at the detector. It is useful to note that over most of the diagnostic energy range 1 μR incident on a 50 % QE detector corresponds to ~ 1 x-ray photon absorbed per 100 x 100 μm pixel. Shown in Fig. 1.3 is a simple radiological model of thickness t, tissue and object attenuation coefficients μ1, μ2 respectively. The object to detect is a cube of dimension x. It can be shown⁶ that the minimum surface dose (energy) D, required to detect the object is given by:

\[
D = \frac{(\mu_{en}/\rho)E_x\kappa t^2(1+R)\exp(\mu_{at})}{QE(\mu_{at}-\mu_{as})^2x^4}
\]

where (μ_en/ρ) is the mass energy attenuation coefficient of the tissue, E_x is the beam energy, k, is Rose's criterion⁷ for detectability (-5) and R is the scatter to primary ratio at the detector plane. The dose required to see detail increases inversely as the fourth power of size of the object (x). It is found that dose starts to become prohibitive above mammographic spatial frequency requirements.

1.3.3 Dynamic range

For a linear response detector, the dynamic range is defined as the ratio of the largest signal at detector saturation to that of the smallest signal detectable above the intrinsic noise floor level of the detector. Although screen-film radiographs have a non-linear response, especially at the lightest and darkest levels of exposure, an x-ray dynamic range of ~ 100 can be assigned to them. Chest radiography and mammography have the largest dynamic range requirements. The
Fig. 1.3: Simplified radiological model used to calculate the minimum amount of radiation required to detect a cubic object of size x. The radiation required increases as the inverse fourth power of x and hence a high frequency resolution limit (small objects) is reached in radiography caused by the biological risk associated with the radiation.
problem of dynamic range in chest radiography has been addressed by scan equalization\textsuperscript{8,9} techniques, the use of high kVp and or large latitude films. The latter two methods reduce image contrast. Recently Philips have introduced a digital a-Se drum\textsuperscript{10,11} chest radiography unit with a large dynamic range. Digital stimulable phosphor systems in theory have a large dynamic range of $10^4$ but in practice may be limited to less than this.

Maidment\textsuperscript{12} et al. estimate that a dynamic range of nearly $10^4$ is required for mammography. It is essential in mammography to use low (20-30) kVp in order to visualize low contrast objects in the breast. In an attempt to deal with the dynamic range problem in screen-film mammography it has become standard practice to compress the breast. It is also argued that compression displaces tissue in a way that allows better visualization of structures. Compression of the breast can be painful and may be a deterrent for some women to have a mammogram. Recently a scanned equalization method for screen-film mammography that has acceptable tube loading has been developed by Sabol\textsuperscript{13,14}.

1.3.4 Detective quantum efficiency

The detective quantum efficiency (DQE) is defined as the ratio $[\text{SNR(out)}/\text{SNR(in)}]^2$ of the output signal to noise ratio (SNR) to the input SNR. The DQE($v,X$) is a function of both spatial frequency $v$ and detector exposure $X$. A DQE of 1 at all relevant $v$ and $X$ indicates the system is perfect. The DQE takes into account how noise as well as signal is transferred in a radiographic imaging system and hence is an objective indicator of how well a radiographic system is performing.

1.3.5 Readout time

Readout time of an image is a purely practical issue. The fastest radiographic film processors now take 45 seconds to perform their function. Therefore it may be stated somewhat arbitrarily that
the readout of a radiographic system image should be about 1 minute or less.

1.4 Inadequacies of present radiological imaging methods

Present radiological techniques, primarily screen-film techniques, suffer from:

- a limited dynamic range, which is especially relevant to mammography and chest radiography.
- an inability to simultaneously achieve high QE and MTF at spatial frequencies above a few lp/mm. A high QE requires a thick screen while only thin screens have a good MTF, hence a high QE and high spatial frequency response are mutually incompatible imaging requirements.
- coupled detection and display (the film) such that both cannot be independently optimized or suitably changed after the radiograph is taken if an exposure error is made.
- an analogue format which causes storage and retrieval problems.
- an inability to conveniently compare radiographs with other images such as CT, MR and US, all of which are in digital format.
- the need to scan films prior to performing automatic computer searches for microcalcifications, or other features, in mammograms.
- a lack of ease to image process films (eg. unsharp masking, Weiner filtering) used to improve image conspicuity.

1.5 Digital radiography

In this thesis digital radiography is considered to involve a detection technique wherein the radiographic receptor forms an electronic signal at the outset which can be digitised. This definition is necessarily "loose" but as an example, digitisation of radiographic films by optical scanning is not considered "digital radiography" per se. Laser scanned read out of photostimulable plates is considered digital since the image readout process is decoupled from the constraints of an intermediate fixed optical storage limitation.

1.6 Approaches to digital radiography using phosphors
Introduction

One general approach to digital radiography is to use an x-ray phosphor to convert x-ray energy to light, which is then detected by a light sensitive electronic detector such as a photomultiplier tube or a CCD. This is a logical extension of the use of phosphors in standard screen-film radiography.

1.6.1 Stimulable phosphors

In screen-film phosphors the fluorescence due to x-ray absorption occurs almost simultaneously with the absorption of x-rays (there may be a slight lag of a few microseconds depending upon the phosphor). The reduction of lag was a problem for early screens as a long afterglow would superimpose one radiograph on a subsequent one. With stimulable phosphors the goal is to enhance lag to the point were the absorbed x-ray energy is stored in trap centres and not released until stimulated by an external light source, eg. a laser beam. The stimulated radiation due to the stored x-ray energy is a different colour from the stimulating readout light thus permitting uncorrupted (by the readout light) detection of the true x-ray signal. Fig. 1.4 shows a schematic depiction of a stimulable phosphor system. This is the only widely available digital radiographic system. Stimulable phosphors do not perform as well as screen-films because only one phosphor screen is used to form the image (due to image alignment difficulties arising in the read out of two screens) rather than two as in screen films. Perhaps for this reason they have not had wide acceptance.

1.6.2 Phosphors optically coupled to CCDs or TV image tubes

A very simple concept has been to minify the optical image of a screen by lenses onto a small CCD or TV vidicon. This approach has been successful for portal imaging applications where dose to the patient is a lesser concern. It is seriously flawed however for radiographic applications
Fig. 1.4: Stimulable phosphor readout. Instead of light being produced at the time of x-ray irradiation the x-ray energy is stored in traps and the image energy is later released by giving it a nudge from a scanning laser beam. The emitted light is a different colour than the laser beam and is detected by a photomultiplier tube (PMT) fibre-optically coupled to the plate. Since it is only practical to use one layer of phosphor instead of two [screen-film systems (Fig. 1.2) use two], stimuable phosphor systems cannot perform as well as screen-film systems.

Fig. 1.5: Coupling the image of a large phosphor screen to a small image sensor is very inefficient using lens systems. Most of the light is not collected by the minifying lens and is wasted leading to a poor DQE.
since the DQE of the system is very low and patient doses must be very high. The poor DQE occurs since only a small fraction of the light emitted by the screen is captured by the imaging lens as is illustrated in Fig. 1.5.

1.6.3 Phosphors fibre optically coupled to CCDs

In an attempt to overcome the poor light collection efficiencies of geometric optics, phosphors have been coupled to CCD area and linear arrays by means of fibre-optics\(^1\). The light collection efficiency is improved somewhat over the lens approach mentioned in the previous section, such that DQE performance starts to approach that of screen-film systems. In addition to the light collection difficulty is the requirement to seamlessly couple a large fraction of a phosphor screen to several CCD detectors. Many CCD detectors are necessary where as the number of discrete elements in a single CCD is less than the number of pixels in a typical digital radiograph. The number of CCDs needed can be reduced by performing slit or slot scans, which has the added advantage of incorporating scatter rejection. However tube loading and image acquisition times are increased.

1.6.4 Phosphors directly coupled to amorphous silicon active matrix arrays

Electronic devices, including CCDs, are almost exclusively based upon c-Si technology and for manufacturing reasons this restricts the devices to small areas. This is because it is difficult and expensive to create a large defect-free crystal and create flawlessly many millions of small elements (~10x10 μm) on the crystal by lithography. An advantage of amorphous materials (materials without long range atomic order, eg. glass is an amorphous material) is the ease with which they can be made into large flat sheets. Recently it has been discovered how to make hydrogenated amorphous silicon (a-Si:H) into a passable semiconductor (and photoconductor).
This has opened up the possibility of large area a-Si:H semiconductor devices comprised of relatively large (~100x100 μm) active devices. Initial interest in a-Si:H stemmed from the desire to make large area inexpensive solar cells. Subsequent to solar cell development, interest in a-Si focused on developing large area active matrix switching arrays for computer flat panel screen displays.

Recently this a-Si:H active matrix switching array technology (developed for flat computer screens) has been adapted for digital radiography. An approach using phosphors is shown in Fig. 1.6. The phosphor acts as an x-ray transducer, converting x-rays to light, which in turn activates photodiodes (one at each pixel). The photodiodes generate charge which is stored on a capacitor and the stored charge can be later addressed and read out. This approach has a fairly high level of complexity (many photolithographic layers are required in the device structure) and it retains the blurring effect of phosphors.

1.7 Direct electrostatic detection

The primary advantage of direct detection (ions or charge) of x-rays by electrostatic rather than phosphor methods is the elimination of image blur. X-rays produce free charge directly in the absorbing electrostatic transducer (solid, gas, liquid) and the charge can be directed by an electric field to a collecting electrode or surface. Because the x-ray signal charge is guided by an electric field the detector can be made very thick to achieve a high QE with almost no loss in MTF or DQE (assuming the read out of image charge at the collecting surface or electrode does not in itself introduce a blurring effect). The idea is presented in Fig. 1.7. It is possible, depending upon the x-ray absorbing transducer, that blurring effects could occur due to k-fluorescence or other effects. For instance this can be a problem when Xenon gas is the detector if resolution above 2 lp/mm is required. Que has theoretically examined such effects for a-Se and predicted that
Fig. 1.6: An active matrix switching array of thin film transistors (TFTs) used to read out image charge created when light from a phosphor screen activates photodiodes, putting charge on the array of storage capacitors. The system inherits the blurring problems of phosphor screens and the TFT, diode array, and storage capacitors make for a complex device.

Fig. 1.7: Direct detection of x-rays using an electrostatic transducer. The image charges, created when x-rays are absorbed in the transducer, are separated and collected by the electric field onto the electrodes of the transducer element or pixel. Since the charge is guided to the electrodes there is almost no blurring.
for diagnostic energy x-rays (18-150 keV) a minimum MTF of 80% is retained at 20 lp/mm even
for a 500 μm thick a-Se detector. A 500 μm thick a-Se detector has nearly 50% QE at 150 keV
and furthermore 20 lp/mm is likely to be more than adequate resolution for all types of radiology,
including mammography.

1.8 Overview of properties of amorphous selenium (a-Se)

It is the high radiographic resolution properties of a-Se in conjunction with its photoconductive
properties (x-rays and light) that make it useful as an x-ray detector and the possible basis for
novel photoconductive readout methods. A-Se has been used as a photoconductor in
photocopiers for more than thirty years and is well developed technologically. Furthermore there
has been a recent revival in the use of a-Se as an x-ray detector and research is under way to
understand and improve its properties as an x-ray transducer. In the remainder of this thesis a-Se
is considered the x-ray photoconductor of choice.

Selenium is element 34 in the periodic table and has two uncompleted bonds in its outer
orbital structure. Selenium can exist in crystalline form but it is the amorphous form (a-Se) which
is of interest for radiography since it can be formed in large uniform sheets. The density of a-Se
is 4.26 g cm⁻³ and due to its relatively low position in the periodic table layers 500 μm thick are
required to absorb about 1/2 of 150 keV photons incident upon it. A-Se is believed to be an
inorganic polymer consisting of covalently bonded chains and although not a crystalline structure
an effective band-gap edge of 2.2 eV can be ascribed to it. There is normally an insignificant
number of free carriers present in the conduction band; indeed the resistivity of a-Se is
exceedingly high at about 10¹⁷ Ω cm. A-Se is a very good insulator unlike c-Si, a semi-conductor,
which has an appreciable number of thermally excited free carriers at room temperature.
Nonetheless a-Se is a photoconductor and light photons more energetic than the band-gap
energy (2.2 eV) create free electron hole pairs, if an electric field is present to separate them. The
photogenerated electrons and holes once separated freely move along the electric field lines and can generate significant currents.

1.8.1 Photogeneration efficiencies

The dielectric constant of a-Se, 6.3, is relatively low compared to other photoconductors such as silicon (12) and germanium (16). According to quantum theory the binding energy of a charge pair (exciton) is given by: 

\[ \frac{-m q^4}{8 e^2 \hbar^2 n^2} \]

where \( m \) is the reduced mass, \( q \) is the electronic charge, \( \varepsilon \) is the dielectric constant of the material, \( n = 1,2,3... \) and \( h \) is Planck's constant. It is because of the high exciton binding energy in a-Se due to a low \( \varepsilon \) (note the inverse square dependence on \( \varepsilon \)) that a-Se has photogeneration efficiency \( \eta \), that is field dependent, unlike the case for germanium and silicon. Pai and Enck\(^\text{22} \) have treated the photogeneration of electrons and holes in a-Se from a classical physics point of view with the one "free" parameter in the model \( r_0 \), the initial separation of the electron and hole after photoexcitation, being equivalent to \( n \) in the quantum model. They applied the three dimensional Onsager model of field assisted thermal dissociation for ion pairs\(^\text{23} \) to a-Se and found \( \eta \) to be given by:

\[ \eta = \theta^{-t_1-t_2} \frac{1}{\xi_2} \sum_{m=0}^{\infty} \frac{\xi_1^m}{m!} \sum_{n=0}^{\infty} \sum_{k-m+n=1}^{\infty} \frac{\xi_2'}{\lambda} \]

where \( \xi_1 = q^5/(\varepsilon_{ae} r_0 k T) \) and \( \xi_2 = q E r_0 (k T) \); \( k \) is Boltzmann's constant, \( T \) the absolute temperature and \( E \) is the externally applied field. The value of \( r_0 \) is 4.5 nm for blue light of wavelength 450 nm. At low values of \( E \) (< 0.5 V \( \mu m^{-1} \)) \( \eta \), according to Eq. 1.2, is nearly independent of \( E \) but as \( E \) increases obeys a sublinear dependence on \( E \) and finally at high fields (\( E > 50 \) V \( \mu m^{-1} \)) again becomes independent of \( E \) when it saturates near unity. It was found experimentally\(^\text{22} \) that at low
values of $E$, $\eta$ was much less than predicted by Eq. 1.2 and in Chapter 3 a qualitative and new quantitative explanation of this is given.

### 1.8.2 Charge carrier (hole and electron) properties

From time of flight (TOF) measurements it has been found that a-Se has well defined electron and hole mobilities; that is electrons and holes move with an average macroscopic velocity that is proportional to the electric field. A typical TOF experiment is shown in Fig. 1.8. It illustrates an idealized sheet of positive charge traversing through a layer of a-Se after a brief ($\ll \tau$ the transit time of the carriers moving across the thickness $d_{se}$ of the a-Se) pulse of blue light created electron-hole pairs at the positively charged surface. The electrons were neutralized at the surface with existing surface positive charges while the freed holes were repelled towards the conductive substrate. The current detected by the transparent electrode is Maxwell's displacement current $\varepsilon_{se}dE/dt$ and is approximately constant during $\tau_p$ (the transit time for holes), provided the amount of freed charge is small compared to the initial amount of charge at the surface. The TOF measurement for electrons is obtained by reversing the polarity arrangements of Fig. 1.8. The mobility of the carriers is given by $\mu = d_{se}/(E\tau)$ where $E$ is the electric field strength in the a-Se layer. The electron and hole mobilities are 0.0063 and 0.18 cm²V⁻¹s⁻¹ respectively.

Electrons and holes have a limited lifetime in the bulk of a-Se due to trapping. The trapping time is dependent upon the presence of impurities or deliberately added elements such as chlorine and arsenic, which can also change the mobilities of carriers. Ideally one would like trapping times to be very long so as to allow for free photoconduction. For well prepared a-Se the trapping times for holes and electrons can exceed 100 μs.
Fig. 1.8: Time of flight (TOF) measurement of the mobility of charge carriers (electrons and holes). One type of carrier is characterized at a time using a proper biasing polarity. Carriers of one charge sign are injected into the bulk of the photoconductor using a pulse of light at the surface of the sample. The pulse of light is much shorter than the time it takes for the carriers to move across the sample thickness. The amount of charge generated in the measurements is small compared to the charge stored on the electrode plates of the sample capacitor so that the electric field will not be weakened (no space-charge effects). During the time the carriers move across the sample the current is constant. The duration of the current pulse can be used to directly measure the mobility of the carriers.
1.8.3 The electric field dependence of \( W_s \)

The amount of x-ray energy \( W_s \), required to create a free electron hole pair in a-Se has a sub-linear field dependence analogous to that of \( \eta \). Que has recently constructed an Onsager theory to explain this observed behaviour by assuming the absorption of x-ray energy creates a distribution of exciton radii rather than a single value as is assumed in Pai and Enck’s treatment of \( \eta \). A typical value of \( W_s \) is 50 eV at \( E = 10 \text{ V} \mu\text{m}^{-1} \) and Fahrig\textsuperscript{24} has shown that the statistical variation of \( W_s \) (the Swank\textsuperscript{25} factor) can be expected to be small. Recently this has been experimentally confirmed by Blevis\textsuperscript{26}.

1.8.4 X-ray interaction processes

The absorption of diagnostic energy x-rays in a-Se is primarily by the photoelectric process at lower energies with the Compton scattering process becoming more important at energies above \( \sim 80 \text{ kEv} \).

1.9 Approaches to digital radiography using electrostatic methods based upon a-Se

1.9.1 Scanning electrometers

The first electrostatic digital radiographic system\textsuperscript{27}, indeed the first digital radiographic prototype, was a scanning electrometer read out of a-Se xeromammographic plates. The essential idea is illustrated in Fig. 1.9. The image surface charge is detected by bringing a conductive probe (and guards), held at ground or virtual ground potential a distance \( d_g \) from the a-Se surface. The surface charge induces charges in the probe in a way which is inversely proportional to \( d_g \). The modulation of the induced charge pattern in the conducting probe held above the image charge rapidly decreases as \( d_g \) is increased according\textsuperscript{28} to: \( \exp(-2\pi v d_g) \), where \( v \) is the spatial frequency.
Fig. 1.9: Electrometer readout of image charge at the surface of a-Se. The magnitude of the induced signal on the probe is inversely related to the separation from the image surface; however the image charge pattern induced in the plane of the electrometer is rapidly (exponentially) blurred as the probe distance is increased. For this latter reason it is difficult to achieve readout resolution greater than 4 lp/mm with this approach.

Fig. 1.10: Active matrix readout using direct electrostatic detection of x-rays by a-Se. The resolution of this approach is limited only by the size of the pixel elements. The practical success of active matrix approaches for radiography is partly related to the manufacturability of large arrays. Active matrix approaches may have a readout noise too large for fluoroscopic applications.
Introduction

of the charge pattern on the surface.

An image of the surface charge is determined by scanning one or several probes over the entire surface of interest. Philips\textsuperscript{11} has developed and commercialized a scanning a-Se drum electrometer system. The drum geometry enables better control of the probe to a-Se surface distance ($d_g$) which is crucial to avoid signal changes related to $d_g$ variations. An AC signal is also applied to the drum which is picked up by the probes and used to calculate $d_g$ so that signal variations due to $d_g$ can be corrected. To achieve high resolution (> 4 lp/mm) the probes must be brought very close to the a-Se surface ($< 100 \mu m$) which introduces the problem of electrostatic discharge\textsuperscript{31} between the probe and a-Se.

1.9.2 Active matrix switching arrays

Instead of using phosphors in conjunction with an active matrix array, Zhao and Rowlands\textsuperscript{29} use a-Se to generate a charge signal, which is collected on a pixel storage capacitor associated with each thin film transistor (CdSe TFT) of the switch array. The concept is shown in Fig. 1.10. Compared to the active matrix phosphor approach (Fig. 1.6) Zhao and Rowlands have replaced the photodiode with a high voltage a-Se diode that interacts directly with the x-ray signal. The resulting structure is less complex than the phosphor-diode approach, doesn't suffer from image blurring, and has a fill factor (active area of pixel) of unity.

1.9.3 Photoinduced discharge (PID) readout

The first PID readout of electrostatic x-ray images was performed at the MD Anderson Hospital in Texas, by Zerneno et al\textsuperscript{30}. The method is illustrated in Fig. 1.11. A latent image is created at the a-Se/(optical-cement,Mylar\textsuperscript{1}) interface and read out by photoinduced discharge through the

\textsuperscript{1} Mylar is a tradename of DuPont.
Fig. 1.11 Laser readout of the MD Anderson duo-dielectric structure. A xeromammographic selenium plate is overlayed with a thin sheet of mylar that has a thin transparent conducting layer of gold evaporated on its upper surface. The mylar and a-Se are considered to form two capacitors in series. The system is charged by applying a bias voltage $V$ while simultaneously being flooded with light. An x-ray exposure is made after the charging process resulting in a latent image charge at the a-Se/mylar interface. The charge is read out by raster scanning a laser beam across the structure. Due to the large capacitance of the structure, image readout noise is also large.

Fig. 1.12: Photoinduced discharge (PID) readout of image charge at an a-Se surface. The induced charge on the transparent readout probe leaves the probe and is detected by a charge amplifier when its associated countercharge on the a-Se surface is discharged through the thickness of the a-Se layer. Since only those induced charges associated with the surface charge discharged by the laser spot are detected the resolution of the system is dictated by the size of the laser spot, which can be made very small (several microns). This approach first demonstrated the high resolution capability of a digital a-Se system and readout noise is lower than the MD Anderson method since the probe capacitance is small. However the readout time is quite long due to the transit time of the charges through the a-Se layer.
a-Se layer. The method proved the principle of PID readout, described in more detail below, but suffered from a high readout noise associated with the large capacitance of the structure. In order to overcome this difficulty and others, an air-gap PID readout method\textsuperscript{31} as illustrated in Fig. 1.12, was devised and tested at the University of Toronto. The incident x-ray intensity field is captured as a latent charge image on the surface of an a-Se plate and read out by discharging, on a pixel by pixel basis with a pulsed laser beam, the surface charge to the underlying conductive substrate. The detection or readout method works as follows: (1) a linear transparent conducting probe is brought near \(d_{\phi}\) the charged free surface of the a-Se which induces counter-charges in the probe, (2) the pulsed laser beam is focused through the probe onto the surface which releases image charges which then travel through the a-Se \(d_{\text{se}}\) to the conductive substrate (photo-induced discharge), (3) as the charges travel through the a-Se (moving further away from the probe) the number of counter-charges (induced-charges) in the probe diminishes (travelling through the charge amplifier) which is detected as the signal.

In the air-gap PID readout method the dimensions of the conducting probe are large compared to the pixel size, which is determined by the laser spot size at the a-Se surface. Although the induced counter-charge in the probe is a blurred representation of that at the a-Se surface, when a region of surface charge is discharged (defined by the laser spot), the signal detected is only due to the countercharges related to discharged surface charge. Therefore the readout resolution is determined by the laser spot size (which can be made very small).

In both the electrometer and air-gap PID readout methods the free surface of the a-Se plate or drum is corotron charged to a uniform potential prior to exposure to x-rays. The potential should be large enough to create an electric field of \(\sim 10 \text{ V \mu m}^{-1}\) in order to reduce \(W_z\) to \(\sim 50 \text{ eV}\). In an electrometer system the residual potential is passively measured; a large remaining offset does not introduce extra noise. However a large remaining bias could cause breakdown between
the probe and a-Se for small $d_g$ required for high resolution. For the air-gap PID system, a standing charge bias remaining after the x-ray exposure reduces charge transit time during photo-discharge but it introduces a discharge noise not correlated with the x-ray signal as will be explained in the next chapter.

1.10 Approaches to overcome air-gap PID limitations

The air-gap PID method is a significant step forward in realizing a high resolution digital radiographic system based upon a-Se. However it has limitations centring around the fixed high bias potential required to make the a-Se layer sensitive to x-rays. We considered arrangements where the air-gap is replaced with a high breakdown field solid-dielectric which would allow flexible insertion and removal of the bias field across the a-Se required to make it sensitive. The use of a solid-dielectric also has the advantage of making an integrated fixed detector with no moving parts, thus eliminating microphonics and allowing for fixed pattern noise removal. Nonetheless we concluded that such approaches would be compromised by long discharge times through the a-Se, especially for a small charge signal, and that a readout bias would have to applied, albeit smaller than for the air-gap PID.

Thus the use of solid dielectrics improve PID readout methods but are intrinsically compromised by the need to move the signal charge through the relatively thick (500 μm) a-Se layer. We wondered if it might be possible to photoconductively switch the signal charge at the a-Se surface a short distance to a conductive readout rail also at the surface? The hypothesis for such an arrangement was that switching or discharging the signal a short distance would reduce readout time over PID methods where discharge occurs through the full thickness of the a-Se. The new surface readout method is called photoconductively activated switched (PAS) readout of a-Se.
1.11 Outline of remainder of thesis

In chapter 2 the operating characteristics of a photoconductively activated switch (PAS) readout method for a-Se is introduced and analyzed. The analysis is carried out using previously known (bulk) photoconductive properties of a-Se. It is found the PAS method can work well in at least two different electrode biasing configurations if the bulk photoconductive properties of a-Se are assumed to hold at the surface.

In chapter 3 experimental results concerning surface photoconductivity of a-Se are presented. The results are quite different from the predictions reached in chapter 2. A theory of surface photoconductivity is developed in chapter 3 which explains quite well all of the experimental results. The theory postulates the existence of deep electron and hole traps at an a-Se/glass interface. This new theory is analogous to surface recombination theories for c-Si but it is demonstrated that for a-Se, surface trapping and not recombination, is the dominant process. The theory explains the departure (at low fields) of the experimental photogeneration efficiency (η) measurements of Pai and Enck from their Onsager theory of η given by Eq. (1.2).

Trapping effects significantly reduce surface photoconductivity in a-Se, making some aspects of the operation of the PAS method as originally envisioned and analyzed in chapter 2, not possible. In chapter 4 it is shown how the PAS method, nevertheless, could work in a light dependent resistive fashion. Additionally different PAS geometries are introduced which could circumnavigate surface trapping effects.

References


Chapter 2

X-ray imaging using amorphous selenium: A novel readout method for digital radiography and fluoroscopy using photoconductively activated switches
2.1 Introduction

A digital radiographic system with a dynamic range, resolution and detective quantum efficiency (DQE) performance better than current screen-film arrangements would confer diagnostic imaging benefits and convenience to radiologists. To date no digital system has been fully accepted clinically. A difficulty in achieving digital radiography is the practical need to make very large area (14' x 17') detectors so that radiographs can be taken quickly and efficiently. Another difficulty is the need to have an appreciable DQE at spatial frequencies as high as 10 lp/mm. Cassette based stimulable phosphor systems provide large area detectors but their DQE performance is less than that of screen-film systems and like other phosphor systems their resolution is limited\(^1\). A selenium based clinical digital chest radiography system has recently been introduced by Philips\(^2\) but it uses an electrostatic probe readout method which does not take full advantage of the high resolution capability inherent in electrostatic selenium approaches\(^3\).

2.2 Success and limitations of PID readout as a motivation for a new photoconductive readout method: PAS

We have previously investigated an air-gap photoinduced discharge (PID) readout method\(^4\) for amorphous selenium (a-Se) and found it to be suitable for high dose, high resolution tasks such as mammography. However an analysis\(^5\) of PID methods for general radiography indicates that it would be difficult to achieve low noise, high DQE and fast readout speed simultaneously due to the requirement of a substantial bias to move the image charges across the thick (500 \(\mu\)m) a-Se detection layer. The bias is most needed at low signal levels and generates an additional signal with an associated noise which compromises x-ray quantum limited detection.

We thought it might be possible to avoid the difficulties of PID approaches if one could
Fig. 2.10(a): Photoc conductively activated switch (PAS) arrangement showing pixel element(s) and readout. The readout is equipped with a transparent non-conductive and an a-Se photoco conductor layer. The charge is collected on the pixel using x-ray signal charge developed throughout the thickness of the detector. In radiographic readout the high voltage (HV) bias is turned off during readout to avoid introducing a bias signal and associated noise.

Fig. 2.10(b): A typical photoinduced discharge (PID) arrangement showing the readout of image charge trapped at the dielectric a-Se interface. X-ray signal charge must be read out by discharging it through the full photoco conductor thickness d2. Typically a large readout bias potential must exist in order to maintain the readout resulting in a large, unwanted, bias signal and associated noise.
photoconductively activated switched (PAS) readout of a-Se

photoconductively read the charge through a shorter distance across the surface of the a-Se. To do this we envisioned the arrangement in Fig. 2.1(a) which shows, in the foreground at the interface of the a-Se detection layer and the transparent dielectric eg. glass, a conducting pixel element (width $d_p$) surrounded by two narrow (width $d_r$) conducting readout rails. The three conducting elements and surrounding photoconductive material constitute a single photoconductively activated switch or PAS. The top surface of the glass is covered with a continuous transparent conducting layer of indium tin oxide (ITO) and the lower surface of the a-Se layer is likewise covered with a thin conductive blocking layer (charges are not injected into the bulk of the a-Se layer) which has negligible x-ray attenuation. The readout rails are maintained at ground potential by their connection to low noise charge detection amplifiers or by a direct connection to ground (Fig. 2.4). A bias is applied to the a-Se and glass electrodes to establish a strong vertical field (10 V $\mu$m$^{-1}$) in the a-Se layer making the layer sensitive to x-rays and moves x-ray generated signal charges vertically to the pixel electrode. The accumulation of x-ray generated charges on the pixel generates a lateral field to the readout rails. Thus signal charge on a PAS pixel can be read out by shining light through the glass onto the a-Se in the region of the lateral field, photogenerating charges in the a-Se, which transfers the signal charge to the readout rail (Fig. 2.1(a), Fig. 2.3). The imaging concept as a whole is illustrated in Fig. 2.2.

2.3 The PAS readout concept: a conceptual evolution of PID

The PAS arrangement is a topological evolution of a typical PID arrangement shown in Fig. 2.1(b). PID arrangements consist of a photoconductor dielectric sandwich with electrodes at surfaces exterior to the photoconductor/dielectric interface. Image charge resides at the interface where it is electrostatically or "capacitively" shared with the photoconductor and dielectric electrodes. Spatially localized readout light is brought in either through the (transparent) dielectric
Photoconductively activated switched (PAS) readout of a-Se

Fig. 2.2: Overview of a PAS digital radiographic or fluorographic system. A laser readout beam activates PAS elements by shining through a transparent dielectric substrate and optical window masks onto the gap between a signal pixel and a readout rail. The PAS detector plate can be integrated into the scanner or inserted into the scanner for readout.
or through a thin transparent photoconductor electrode. In either case the image interface charge is read out by discharging it through the bulk of the photoconductive layer ("bulk" means the interior of the photoconductor away from its surfaces). The key to developing the largest signal in the PID approaches is to share equally the signal charge between the top dielectric electrode \((C_u)\) and the bottom photoconductive electrode \((C_{se})\). In contrast if most of the capacitance is in the photoconductive layer virtually no signal will be detected since the discharge process is essentially an internal neutralization process. The ratio of the maximum detectable signal charge readout to the image surface charge is defined as \(\Lambda_c\), and is given by: \(C_s/(C_{se}+C_e)\) under the assumption that the image charge is completely discharged. In the PAS arrangement of Fig. 2.1(a) the image charge of the pixel element is principally coupled (capacitively) to the adjacent readout rails because the rails are so close to the pixel. Thus the capacitances to the top dielectric and bottom photoconductive bias electrodes are of minor importance. Pixel readout may be accomplished by a charge transfer process between one of the readout rails and the pixel. The capacitances to the pixel electrode of the left and right readout rails are \(C_u\) and \(C_r\), respectively and are equivalent to \(C_{se}\) and \(C_e\) of PID arrangements. The pixel capacitance to the biasing electrodes is \(C_{be}\), and \(C_{be} << C_r\) or \(C_u\). The signal coupling efficiency \(\Lambda_c\) is then given by:

\[
\Lambda_c = \frac{C_{be}}{C_{se}+C_e+2C_{be}}
\]

where complete discharge via continuous illumination through \(C_u\) is assumed. If the arrangement is symmetric and \(C_{se}=C_e\) then \(\Lambda_c \approx 1/2\).

The bulk mobility of holes \((0.18 \text{ cm}^2\text{V}^{-1}\text{s}^{-1})\) in a-Se is about 28 times that of electrons\(^6\,^7\). Therefore it would be advantageous to use only holes in the operation of a PAS. This could be accomplished by shining readout light close to the more positive electrode of the rail pixel gap
as shown in Fig. 2.3. In a general analysis\(^5\) for the PID method the fastest readout time is achieved by using a pulse shorter than the transit time of holes across the readout junction. In this pulsed mode of operation only the fraction \(F = \frac{C_n}{C_n + C_r + C_{be}}\) of the charge is read (discharged) but advantageously the remaining "unread charge" contributes to the field across the junction resulting in a faster readout time. The fastest pulsed-light readout has been shown to occur\(^5\) in PID arrangements when \(C_{se}\) and \(C_c\) (ie. \(C_r = C_n\)) are equal. A similar principle could be expected to occur in the PAS arrangement but the details might be different due to the different geometry and action of the electric fields. For pulsed illumination the ratio \(\Lambda_p\) of the signal detected to the total image charge in the PAS arrangement is given by the product of \(F\) and \(\Lambda_c\):

\[
\Lambda_p = \frac{C_n C_r}{(C_r + C_n + C_{be})^2}
\]  

Unless stated otherwise it is subsequently assumed that all readout operations are of the short pulse type, \(C_r = C_m\), \(C_{be} = 0\) (hence \(\Lambda_p = 1/4\)) and that the readout time for this condition is not far from optimal.

### 2.4 PAS readout operation

When a PAS pixel is switched by pulsing light on one of the rail/pixel gaps, current signals of equal and opposite polarity develop on the two rails adjacent to the pixel. Consider, for example, a signal of eight positive charges on the floating signal pixel coupled to the rails at ground potential as shown in Fig. 2.3. A narrow, but intense strip of light is pulsed at the left edge of the signal pixel. The number of photocharge generated electron-hole pairs (ehp) will equal or exceed the number of negative countercharges (four) in the left rail. The electrons will neutralize the four
Fig. 2.3: A simplified account of how a signal is generated in a PAS element by capacitive sharing of the image charge on the pixel and two neighbouring readout rails. Readout light for each PAS element is shone in only one of the pixel readout rail gaps. As shown here the neutralisation of charge in the left rail by a brief pulse of readout light (compared to charge transit times across the gap) is followed by a redistribution of charge on the pixel which develops a signal of equal and opposite magnitude on the two readout rails.
positive charges leaving four holes to traverse the gap and ultimately discharge or neutralize four electrons on the left rail. Any excess ehp recombine. However, during the time the holes move across the gap, a redistribution of positive charge on the pixel occurs ultimately bringing two positive charges to the left side of the pixel (leaving two on the right side). The presence of the two positive charges is matched by two "new" electrons which move into the left signal rail since it is at (virtual) ground. For the right rail, after redistribution, the amount of positive charge has been reduced by half, therefore two "old" negative charges must flow out of the right rail and hence a negative signal is created.

Two separate issues must be considered during readout. First, when switching a pixel it must be arranged such that light discharges only one of the pixel rail gaps, as equal illumination of both gaps would lead to a null signal. Second, reading even and odd pixels simultaneously mixes the signals of neighbouring pixels (the readout rails are shared) which is further compounded by the fact that the signals have opposite polarities. Thus a uniform image readout in this way would result in signal cancellation. Therefore each row must be read out twice, first reading odd pixels and then reading out even pixels. This approach is shown in Fig. 2.4, where optical masks have been employed to select light from a narrow scanning fan beam whose width is less than a 1/2 pixel.

2.5 Reconciliation in a PAS element of the vertical field requirements for x-ray signal collection and the lateral field requirements for signal readout

Is it possible in the PAS arrangement to have both a vertical field to collect signal charges on the pixels while also having a horizontal field to readout signals from the pixel to the readout rail? In the next section(s) the behaviour of the electric field in the readout gap and bulk of the a-Se layer
Fig. 2.4: One method of reading alternate pixels to eliminate signal mixing. A scanning line of light moves vertically over the PAS array initiating charge switching only when it passes through optical windows onto a PAS element. Only half of the pixels of a row can be readout simultaneously.
is discussed as an x-ray charge signal is accumulated on a pixel. Two biasing schemes (1. *radiographic* and 2. *fluoroscopic*) are proposed to minimize the conflicting requirement of a vertical field for charge collection and a horizontal field for charge readout: (1) A unidirectional vertical bias field in both the a-Se and dielectric layers is simply turned off during readout (2) a bi-directional bias field (pointing in one direction in the a-Se layer and the opposite direction in the dielectric layer) can be established in such a manner as to effectively null out the vertical bias component in the readout gap.

2.5.1 The *radiographic* mode

The Fig. 2.5 sequence shows the behaviour of field lines as an x-ray signal is accumulated for a bipolar biasing situation with the top glass electrode negative and the bottom a-Se electrode positive. Initially as shown in Fig. 2.5(a), with no residual charge on the pixel electrode, the field would be purely vertical which is optimal for signal collection. Subsequent diagrams concentrate on the ROI defined in Fig. 2.5(a). In Fig. 2.5(b) enough x-ray generated charge has accumulated on the pixel to introduce a field distortion near the rail-pixel gap but it is insufficient to create a strong enough horizontal field to establish field line coupling from the pixel to the rail. In Fig. 2.5(c) the critical amount of charge has been deposited on the pixel to establish a strong enough horizontal field such that readout light would transfer charge from the pixel to the readout rail rather than to the bottom a-Se bias electrode. The requirement of a minimum threshold exposure level for readout is removed by switching the bias off, as shown in Fig. 2.5(d), for readout. Then x-ray charge on the pixel electrode creates a purely lateral field component at the plane of the junction. Thus charge can be moved across the junction even for small signal charges. We refer to the mode of operation where a bipolar bias is turned off during readout the *radiographic mode* of operation as it is most suitable for single radiographs.
Fig. 2.5(a): Pixel geometry model used for field calculations of PAS operation. Bias electrode polarities are for the radiographic mode of operation; the rails are at virtual ground potential, the pixels are "floating" and with no signal yet collected on any pixels the field lines are purely vertical. The field lines for the boxed region of interest (ROI) are shown in (b), (c) and (d) for increasing amounts of x-ray irradiation. (b): ROI field lines after 10 mR exposure; field lines do not connect pixel and rail electrodes; radiographic bias still applied. In this and following diagrams the local x and y coordinates (in microns) of the model are shown. (c): ROI field lines after 30 mR exposure; field lines connect pixel and rail; charge transfer possible without switching radiographic bias off. (c): ROI field lines after 1 mR exposure with bias turned off.
2.5.2 The fluoroscopic mode

In fluoroscopy the x-ray irradiation is on continuously. Thus it is necessary to have the bias on continuously, so as to ensure that all the x-ray induced charge is collected. However a bias arrangement must be found that would not introduce a vertical field component in the readout junction which would otherwise: (a) compromise pixel switching by moving signal charges vertically into the bulk rather than horizontally to the adjacent readout rail and (b) introduce a bias signal by the photogeneration of readout charges that would move to the a-Se electrode. In Fig. 2.6(a) we illustrate a unipolar biasing scheme which should achieve this end. A positive bias is applied to both bias electrodes and with the pixel electrodes initially charge neutral. The pixel electrode will assume a potential intermediate between the ground potential of the readout electrodes and the positive potential of the biasing electrodes. This results in a large unwanted field between the readout rails and the pixels. However by shining light at the readout junctions negative charge will be transported to the pixel electrodes bringing them to a potential very near that of the readout rails so that at this point the lateral field is almost zero (Fig. 2.6(b)). The system is now initialized and ready to acquire a sequence of fluoroscopic images.

When x-rays are incident on the a-Se, the charges they generate are principally collected on the pixel electrode which starts bringing it back to a more positive potential. The field arrangement moves qualitatively to the type shown in Fig. 2.6(a) i.e. a horizontal field, proportional to the x-ray signal, develops between the pixel and the readout rails. The x-ray charge can then be read out without turning the bias off by shining the readout light in one of the readout junctions as was done to initialize the system. This is the fluoroscopic mode of operation and it can be thought of as a recharge operation since the pixel electrode must be recharged to its equilibrium negative charge state at the end of each readout operation. When operating in the fluoroscopic
Fig. 2.6(a): In the fluorographic biasing arrangement both the a-Se and dielectric biasing electrodes are positive. Initially this induces a large horizontal field in the pixel rail gap and the field in the a-Se deviates quite significantly from being purely vertical.

Fig. 2.6(b): By applying "initialization" scans in the pixel rail gap negative charge is transferred to the pixel elements bringing them to a potential near that of the rails (ground), the lateral gap field is gone and the a-Se field is nearly vertical; the system is ready to acquire image(s) with the x-ray bias on at all times. Accumulation of positive x-ray generated signal charge on a pixel moves the field configuration qualitatively back to that of Fig. 2.6(a).
mode considerable frame to frame lag can exist since only half the signal charge is annulled each time a scan occurs. However this is often an advantage and an equivalent process is often introduced in digital fluoroscopic noise reduction systems. Alternatively pixel readout lag can be reduced to an arbitrary low value by multiple readouts (e.g. to minimize lag to 2% one would require \( \log_4(0.02)/\log_4(0.5) \approx 6 \) scans per image frame).

2.6 Calculation of Device Performance

In order to analyze the behaviour and performance of the PAS method, a general method is needed to calculate electric potentials, fields, capacitances and other parameters as the biasing and geometric configurations are altered. It would be useful to calculate how the electric field of the system changes during the generation of the x-ray signal when charge is collected on the pixels so that the characteristic curve (signal vs. x-ray exposure) of the method can be found. Capacitances of the electrode structures are required in order to calculate readout noise of the system. Knowledge of the readout noise and characteristic curve then allows the determination of the dynamic range. The dynamics of idealized photogenerated charge transfer across the readout gap is also sought to compare to experimental photocurrent measurements.

We also need to get an estimate of cross-talk between pixels to estimate resolution losses. As shown by Que\(^3\) the intrinsic x-ray signal detection modulation transfer function of a-Se is very high even for thick layers with high quantum efficiency. For instance for a 500 \( \mu \)m thick a-Se layer at an x-ray energy of 50 keV the MTF has dropped to only 80% at a spatial frequency of 20 lp/mm. In the PAS readout method the electrostatic field configuration will ensure that charge generated beneath a pixel will be collected only on that pixel. Although it is expected that the resolution of the system will be principally determined by the sampling pitch, resolution could be compromised on readout by electrostatic field cross-talk effects.
Thus we need to solve the electrostatic fields pertinent to our problem both for static situations and for quasi-dynamic situations involving the time evolution of the solutions during an x-ray exposure and the optical readout of charge. From the field strengths used and the carrier mobilities for a-Se, the macroscopic movement of charge in a-Se is so slow \((v = \mu E \sim \text{velocity of sound in air})\) as compared to light velocities that the electrodynamics reduce to the solution of Maxwell's equations without magnetic field effects: in other words to time series solutions of electrostatic fields.

One could rely on commercial software, which is invariably based upon finite element methods. However difficulties or limitations may be encountered when trying to solve a sequence of field solutions that must be coupled to user external equations and parameters not directly related to electrostatics, ie. x-ray interactions and photogeneration of space-charge. Finite element software is very complicated, especially the mesh generation algorithms, and the wisdom of writing one's own finite element package seems questionable. We decided to use an integral method of solving electrostatics that has an intuitive physical basis, is very simple, fast, and easy to implement. We have thus been able to solve the electrostatic fields in a straightforward manner and thus study the time dependent effects of space-charge generation resulting from both the interaction of x-rays and of light in the a-Se layer.

2.6.1 Charge simulation modelling (CSIM)

The integral field solution technique used is the charge simulation method (CSIM) discussed by Haus and Melcher\(^8\) and in more mathematical detail by Harrington\(^9\). It is similar to boundary integral methods\(^11\) and is founded on a fundamental theorem from electrostatics for conductors which states that the macroscopic space-charge density in the interior of a conductor must be zero everywhere and that the net static charge on a conductor must reside on its surface\(^12\). A
corollary to this is that a conductor, when subjected to the presence of an external field, will arrange charge densities on its surface to null the interior electric field to zero. We can use these facts to solve electrostatic field problems by modelling conductors as surfaces comprised of a number of small charge elements or strips which have the appropriate amounts of charge on the strips to maintain an equipotential. As the electrodes are divided into finer strips the solution approaches the exact solution.

For illustrative purposes we now give a conceptual description of the CSIM method for solving the fields for a parallel plate capacitor (the full solution method used for solving the PAS electric fields is given in Appendix 2.1). Shown in Fig. 2.7 is a parallel plate capacitor (extending infinitely in and out of the plane of the paper) which has been divided into N smaller charge strips each with a uniform charge density \( \sigma_i \) (i=1,...,N) and width \( a \). Each strip is part of one of the capacitor electrodes and is considered to be of infinitesimally small thickness. A mathematical convention describing the potential of any strip is required. Consider for the moment the potential generated by a strip with charge density \( \sigma \) located at the origin \((0,0)\). The potential \( \Phi(x,y) \) (at an arbitrary point \( x,y \)) due to the strip can be given as:

\[
\Phi(x,y) = G(x,y)\sigma
\]

(2.3)

where \( G \) is the known (Appendix 2.1) source or generating function describing the potential for the charge sheet. If the strip is now translated to the location \( X,Y \) the potential is given by \( \Phi(x,y) = G(x-X,y-Y)\sigma \). Returning now to the capacitor, the potential due to each of its strips \( \sigma_i \), centres located at \( (X_i,Y_i) \), is given by \( \Phi_i(x,y) = G_i(x-X_i,y-Y_i)\sigma_i \). Instead of considering the potential at an arbitrary point \( x,y \) in space now consider the potentials specifically at the centre of the strips, where boundary conditions exist. At the centre of the \( j^{th} \) strip (we introduce a new dummy index \( j \) for reasons soon apparent) the total potential at that location must take into consideration the
Fig. 2.7: Illustration of charge simulation method (CSIM) applied to a parallel plate capacitor consisting of two plates that extend infinitely in and out of the plane of the paper. The plates are assumed to have zero thickness, although for illustration purposes they are shown with a thickness. The plates are divided into a finite number N of charge strips of width a. The charge densities of all the strips are adjusted so that the potential along the top and bottom plates are $V/2$ and $-V/2$ respectively.
contribution from the strip itself and all the remaining other strips (by the superposition principle). This is represented mathematically by stating that for each strip \( j \) \((j=1,\ldots,N)\) the total potential \( V_j \) is given as:

\[
V_j = \sum_{i=1}^{N} G_j \rho_i
\]  

(2.4)

where \( G_j = G(x_j-x_i, y_j-y_i) \) and \( i=1,\ldots,N \). If we adopt the repeated index summation convention (wherever in any term of an expression an index occurs twice this term is to be summed over all possible values of that index) we have:

\[
V_j = G_j \rho_j
\]  

(2.5)

where \( V_j \) is the potential of the \( j^{th} \) charge strip and is normally specified by the boundary conditions. For instance in Fig. 2.7 the strips from 1 to \( N/2 \) all have the same positive potential \( V/2 \) and the strips from \((N/2)+1\) to \( N \) all have the same negative potential \(-V/2\). The above Eqs. (2.5) can be viewed as a matrix:

\[
\begin{bmatrix}
V_1 \\
\vdots \\
V_N
\end{bmatrix} =
\begin{bmatrix}
G_{11} & G_{12} & \cdots \\
G_{21} & \ddots & \vdots \\
\vdots \\
G_{NN}
\end{bmatrix}
\begin{bmatrix}
\sigma_1 \\
\vdots \\
\sigma_N
\end{bmatrix}
\]

where the potential vector on the left hand side of the Equation is known, the source functions \( G \) are known, and the unknown vector of charge densities is solved for by linear algebra methods. In the parallel plate example one will find more charge near the ends of the electrodes as it is
necessary to shore-up the potential there due to the lack of contributing neighbours. Physically this occurs because charge will flow until the potential gradient or force on the charges is reduced to zero.

In the above example the field solution is two dimensional (2D) since the field varies in x,y but not z. Note however that the 2D CSIM field solution only requires the solution of charge densities in one dimension i.e. along the lines of the electrodes thus reducing the dimensionality of the problem by one. A finite element solution to the same problem would have required dividing the x-y plane of the solution space into planar elements and also required the imposition of additional (beyond the specification of the potentials of the electrodes) boundary conditions at arbitrary exterior surfaces to the solution space.

If the potential is not known of an electrode, i.e. it is floating, then an auxiliary equation concerning the net charge of all the charge strips comprising the electrode is needed which will make the system of linear equations solvable. Also as described in Appendix 2.1 the charge neutrality of the entire solution system must be maintained. Once the charge density vector is solved the potential and hence electric field can be calculated at any point in space. Note that both the rails and pixels are treated as infinitely long in the modelling which is a good approximation in a real device where the rails may be 5 μm wide and 20 cm long. The approximation is also quite good for the pixels which may be separated from the rails by a distance of only 5μm but have a perimeter of 400 μm. The capacitance of a pixel is calculated by simply multiplying its length by the capacitance per unit length of the pixel strip in the model.

With a solution method of electric fields at hand we now proceed to apply the method to enhance understanding of the operation of the PAS method.

### 2.6.2 X-ray calculations
The amount of charge collected on a pixel vs. x-ray exposure $X$, was determined in discrete exposure steps $\delta X$ (mR). The fields were recalculated for each successive increment of exposure. Even after a large (100 mR) x-ray exposure the magnitude of the electric field throughout the a-Se bulk was found to be quite uniform, especially near the substrate where the x-rays enter and are primarily attenuated. Contours of equal field magnitude are shown in Fig. 2.12(b) to illustrate this point. Therefore a good approximation of the a-Se x-ray sensitivity $W_\pm$ at each step was determined by calculating the electric field at the centre of a pixel element and the middle of the a-Se layer by applying the empirical formula:

$$W_\pm = k' |E|^{-n}$$ \hspace{1cm} (2.6)

where $W_\pm$ is the energy in eV required to create a free ehp, $k'$ and $n$ are empirical constants and $E$ the electric field. To determine the incremental amount energy $\delta W$ absorbed in the a-Se the following formula was used:

$$\delta W = \delta W_{inc}(1 - e^{-\mu_{abs}d})$$ \hspace{1cm} (2.7)

with $W_{inc}$ the incident energy and $\mu_{abs}$ the energy absorption coefficient at x-ray energy $E_x$ (The predictions of Eq. (2.7) have been compared to Monte-Carlo calculations in the diagnostic energy range and have been found to agree within a few percent). The x-ray spectrum\textsuperscript{13} used was monochromatic with an x-ray energy $E_x$ of 35 keV, nearly equivalent to a polychromatic spectrum obtained from a 2 mm Al filtered 70 kVp tungsten bremsstrahlung x-ray tube output. The incident number of quanta was $2 \times 10^5$ photons mR$^{-1}$mm$^{-2}$.

The behaviour of the electric field lines as a function of $X$ was quantified to determine what fraction of generated charges were collected on the pixel electrode. This was done by calculating
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field lines, at each exposure level, from the centre of the a-Se layer, to the a-Se/glass interface. Those lines which terminated on the pixel electrode would transfer charge from the central region of the a-Se to the pixel. The left most and right most coordinates away from the central x position of the pixel electrode then defined a charge collection volume $c_v(X)$, always smaller than the pixel pitch volume $p_v$. The differential ($\delta X$) charge collection efficiency DCE($X$) is then defined as $c_v(X)/p_v$. The DCE($X$) is the percentage of charges collected on a pixel from the $p_v$ at an accumulated exposure $X$ for a small incremental exposure $\delta X$. Strictly speaking the calculation should determine what fraction of charges generated at each depth ($y$ coordinate) of the a-Se follows field lines to the pixel. However as can be seen in Fig. 2.12(a) even with a large exposure the field lines only deviate significantly from a vertical direction near the a-Se/glass interface where they turn and start to terminate on the readout rails, reducing the charge collection efficiency. Furthermore since most of the x-rays are absorbed in the bottom layer of the a-Se most of the x-ray generated charge is produced in the lower half of the a-Se layer where the field lines, showing very little perturbation from the vertical direction, guide them to the central region of the layer where the DCE($X$) calculations begin.

2.6.3 Photoconductive readout current calculations

The readout signal current was calculated by introducing equal numbers of positive and negative line charges, which have potentials as given by Eq. (2.15), in the rail-pixel gap at the a-Se glass interface, simulating the action of blue light. The results of this type of calculation were of particular interest as the starting point in understanding the experimental current measurements described in chapter three. The amount of space-charge introduced ranged from $\sim 1/30$ to almost one half of the amount stored on the pixel and was introduced at varying positions in the gap. In order to prevent immediate recombination of carriers of opposite sign at the interface layer (the
charges move laterally and in opposite directions and in the model are created in an infinitesimally thin layer) charges of opposite sign were given a small vertical (y) displacement away from each other. The current J is then given by:

\[ J = \epsilon_{se} \frac{\partial E}{\partial t} q \mu_n n E + q \mu_p p E \]  

(2.8)

where the first term is Maxwell's displacement current (\( \epsilon_{se} \) is the dielectric constant of a-Se) while the second and third terms are due to the movement of physical carriers (\( \mu_n, \mu_p, n, p \) are the electron and hole mobilities and densities; q is the fundamental unit of charge). The above equation was implemented at a readout electrode as follows:

\[ J(t) = \frac{Q_{ei}(t) - Q_{ei}(t-\delta t)}{\delta t} - \frac{Q_{sp}(t)}{\delta t} \]  

(2.9)

where the first term is the change in the electrode charge \( Q_{ei} \) during \( \delta t \) and is equivalent to the displacement current \( (\epsilon_{se} \frac{\partial E}{\partial t}) \) while the last term is the physical amount of space-charge \( Q_{sp}(q \mu_n n E + q \mu_p p E) \), reaching the electrode per unit time.

2.6.4 Field modelling results

All the field profiles, capacitances, and currents in this chapter were calculated with the CSIM methods described in Appendix 2.1. Figs. 2.5 and 2.6 used the pixel geometry shown in Fig. 2.1(a): \( d_{se} = d_e = 300 \mu m \) thick, \( d_p = 100 \mu m, d_i = 10 \mu m, d_g = 5 \mu m \) resulting in a pixel pitch \( (d_p + 2d_g + d_i) \) of 120 \mu m. The dielectric constant of the transparent layer (glass) was set equal to
Fig. 2.8(a): The electric field magnitude across a 254 μm gap between two 254 μm electrodes (the two rail geometry). The potential difference of the electrodes was 1000 V; the electrodes are infinitely thin which in principle generates a field of infinite strength at the electrode edges.

Fig. 2.8(b): The electric field magnitude across a 5 μm gap in the pixel geometry (see ROI in Fig. 2.5(a)). The field is due to the accumulated charge on a signal pixel after 1 mR of exposure and there is no bias present on the a-Se or transparent dielectric bias electrodes. The charge on the other pixels is zero. The field profile is not perfectly symmetrical due to the effects of the gap on the other side of the rail. The slight negative undershoot of the field is due to the nature of the finite derivative.
Fig. 2.9: The capacitance of two rails, each width $d_r$, separated by a gap $d_g$ (two rail geometry). This is a good approximation to the capacitance behaviour of the rail and pixel of Fig. 1(a). A reasonable guess to the capacitance of the two rail geometry might be to suppose $C = \left(\frac{d_r}{d_g}\right) \varepsilon_0 \varepsilon_{se}$, but in fact this is seen to overestimate the capacitance at small $d_r/d_g$ ratios and underestimate it at large ratios.

Fig. 2.10: Ignoring space-charge effects the pixel readout time for a 100 $\times$ 100 $\mu$m pixel separated from a 10 $\mu$m rail by a 5 $\mu$m gap (pixel geometry). The x-ray spectrum was 70 kVp filtered by 2 mm Al. To simplify calculations the gap field was considered to be uniform and holes were assumed to be the charge carriers across the full width of the gap. If the readout rails are given a 1 or 0.1 Volt bias during readout the readout time can be kept to ~1 or 10 $\mu$s respectively for all exposures.
Fig. 2.11: The calculated differential charge collection efficiency (points) for the pixel geometry and a 70 kVp 2 mm Al filtered spectrum. The differential charge collection efficiency (% of signal charges collected on the pixel for a small incremental exposure) drops off rapidly at large exposures as the signal charges steer electric field lines away from the pixel (Fig. 2.12(a)).
that of a-Se, i.e. 6.3. There were five PAS elements and the results are from the left pixel-rail gap of the third (central) element.

The field profile shown in Fig. 2.8(a) and readout currents of Fig. 2.14 (a) and (b) were calculated with a *two rail geometry*: two isolated rails of 254 μm width (d,), separated by a gap (d,g) of 254 μm. Fig. 2.9 shows the capacitance calculated using the *two rail geometry* as a function of the rail/gap ratio. Also plotted in Fig. 2.9 is an estimate of the capacitance of the two rail geometry assuming C = ε₀(d/d,g).

The electric field as a function of gap position (Fig. 2.8(b)), the differential charge collection efficiency as a function of exposure (Fig. 2.11), the field line behaviour for a 100 mR exposure (Fig. 2.12(a)), contours of equal field magnitude (Fig. 2.12(b)) and the characteristic curve (Fig. 2.13) were all calculated using the *pixel geometry*. It should be noted that in *radiographic mode* calculations using the bipolar bias, +3000 V was applied to the a-Se bias electrode and -3000 V to the glass bias electrode yielding a total potential difference of 6000 V across the entire structure during the x-ray exposure; the bias was removed for readout. A unipolar bias of +3000 V was applied to both the a-Se and glass bias electrodes in the *fluoroscopic mode* calculations.

In Fig. 2.9 the capacitance of the *two rail geometry* is shown as a function of the ratio of the gap to rail/pixel width. The pixel readout time vs. exposure shown in Fig. 2.10 was calculated assuming the more mobile holes were created near the pixel electrode edge and moved across the gap width to the readout rail. For this calculation the gap field was taken as the mean value and independent of position. The readout time is calculated with and without a 1 V standing bias added to the gap in addition to the signal potential. In practice the readout bias would be applied by reducing the voltage of the rails from ground to negative one volt during readout. From Fig. 2.10 we find that a 1 V bias is sufficient to assure a minimum readout time of ~1 μs even at low
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Fig. 2.12(a): Graphic illustration of how field lines steer away from a pixel electrode after it has accumulated a signal charge (100 mR exposure). The field lines from the a-Se bias electrode bend away from the pixel when they get near the plane of the a-Se/transparent dielectric interface.

Fig. 2.12(B): Contours of equal field strength after a 100 mR exposure. There is a variation of field strength in the region near the rails and pixel, but the field strength is nearly constant in the bulk of the a-Se where the x-rays interact. This observation justifies using the field strength at the central y coordinate of the a-Se (y=150 microns) to calculate the x-ray sensitivity.
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exposure levels.

The differential charge collection efficiency DCE(X), for the pixel geometry is plotted in Fig. 2.11. The two dimensional electric field profile is shown in Fig. 2.12(a) after a large (100 mR) exposure with the bias still applied and Fig. 2.12(b) shows a contour plot of the field magnitude. The characteristic curve of the PAS system (pixel geometry), the amount of charge collected on a pixel as function of X, is shown in Fig. 2.13.

Readout current calculations were performed with a simulated narrow band of pulsed light shining in an asymmetric position near one of the rail electrodes in the two rail geometry (shown in the inserts of Fig. 2.14(a) and (b)) or by the pixel electrode in the pixel geometry (see insert Fig. 2.14(d)). In both models the band of light was 40 μm wide and the gap, rail and pixel electrode widths were 254 μm (chosen to conform with experimental arrangements reported in chapter 3). The potential difference across the gap was maintained constant for the results of Fig. 2.14(a) and (b), again to be in accordance with experimental conditions. In Fig. 2.14 (c) the pixel electrode was floating with an initial amount of positive charge (on the pixel while the rails and substrate electrodes were maintained at zero Volts. In all readout current calculations, bulk drift mobilities and infinite carrier lifetimes were assumed (i.e. trapping effects at the surface were not included (see chapter 3)). We define significant space-charge in the region of an electrode as that which is the same order of magnitude as the charge stored on the electrode itself. The hallmark of significant space-charge is a distortion of the electric field from the field configuration without space-charge. Insignificant space-charge is at least an order of magnitude less than the charge stored on the electrode.

The photocurrents arising from the use of low light levels (generating insignificant space-charge) and high light levels (significant space-charge) with the light shining near the positive electrode are shown in Fig. 2.14 (a) and the result for the reversed polarity in Fig. 2.14 (b). In the
Fig. 2.13: The characteristic curve (pixel charge signal as a function of x-ray exposure) of the PAS readout method is plotted both as the charge per pixel (left axis) and as the gap field (right axis) as a function of x-ray exposure. The dielectric strength of a-Se is \( \sim 100 \text{ V/\mu m} \) (horizontal line), therefore breakdown effects could be expected at an exposure of \( \sim 350 \text{ mR} \).
Photoconductively activated switched (PAS) readout of a-Se

Gap = 254 μm  E = 3 V/μm

Curve A (10 X current)

Curve B

Hole current

Electron current

Fig. 2.14(a): The current signal that could be expected by shining a brief (<< the transit time of holes across the gap) pulse of light in the gap near one of the electrodes in the two rail geometry (254 μm gap) maintained at a potential difference of 762 Volts. The electrode polarities and position of the beam (width 40 μm, centre 30 μm from edge of electrode) are so chosen to make holes traverse the width of the gap. Two different amounts of space-charge were chosen to be generated by the light pulse: 1/30 (curve A) and 1/3 (curve B) of the amount of charge stored on the rails. The signal resulting from the weak pulse of light (curve A) has been multiplied by ten in order to compare it with the brighter signal.

Fig. 2.14(b): The current signal resulting with a polarity opposite to the conditions in Fig. 2.14(a). The initial burst of current is due to the holes moving a short distance to the cathode. After the burst of hole current electrons traverse the width of the gap generating a weaker prolonged current for about 130 μs. The same amounts of space-charge were used as in Fig. 2.14(a), but the effects of a larger space-charge are not significant during the time plotted.
Charged pixel readout

Readout beam

Rail

Pixel

Selenium

Time (μs)

Current (A m⁻¹)

0.0

5.0x10⁻⁴

1.0x10⁻³

1.5x10⁻³

2.0x10⁻³

2.5x10⁻³

Fig. 2.14(c) Charge transfer between a floating charged pixel (pixel geometry) and rail maintained at ground potential. The rails, gap and pixel are all 254 microns. Curve A (current x 10) is for an amount of space-charge that does not much effect the gap field whereas curve B involves an amount of space-charge comparable to that stored on the left rail. The larger space-charge collapses the field in the region of its presence during the first few microseconds and later as charge reaches both the pixel and rails the fields weaken further. However since the pixel has charged stored on the other rail the field at the end of the discharge process has been reduced to about half its initial value.
first case holes traverse practically the whole gap (~ 210 μm) in a time (~7 μs) less than it takes the electrons to saunter ~30 μm into the adjacent positive electrode. Under these circumstances readout is fastest as the holes are much more mobile than electrons and contribute to most of the charge transfer (jτdt). Conversely with the polarity reversed (Fig. 2.14 (b)) the electrons contribute a large fraction of the charge transfer, but over a much longer period of time (~ 130 μs), as they must travel nearly over the entire gap. In the first microsecond the holes quickly move to the negative electrode (generating the brief initial current pulse) and are neutralized.

2.6.5 Readout noise considerations

As in all clinical x-ray imaging systems it is very desirable that x-ray quantum noise be the dominant noise source at all spatial frequencies and x-ray exposures encountered clinically. The x-ray quantum noise per pixel is given by:

\[ N_x = g \sqrt{\phi_x} \]  

(2.10)

where \( \phi_x \) is the average number of absorbed x-ray quanta per pixel, and \( g \) is the effective gain of the system given by \( g = (W_x/W_p)A_p \).

The charge amplifier contributes the constant noise \( N_A \) (expressed in units of \( q \), the fundamental unit of charge) which is given by:

\[ N_A = \kappa + \kappa' C_R \]  

(2.11)

where typical values of \( \kappa \) and \( \kappa' \) are 80 \( q \) and 3 \( q/pF \) respectively. \( C_R \), the total readout capacitance, depends primarily on the pixel/rail gap and the size (length) of the detector.

As device size is scaled up, the second term in Eq. (2.11) can become a problem. The
capacitance of a rail surrounded on two sides by pixels 100 µm wide separated by gaps 5 µm on each side can be estimated from Fig. 2.9. The plate separation/plate width ratio is 0.05 which yields a capacitance of 175 pFm⁻¹. Since the rail has capacitance to two rows of pixels the capacitance must be multiplied by two yielding 350 pFm⁻¹.

There will be thermal noise associated with the charge on the pixel/rail electrode capacitance C given by:

\[ N_{kTc} = \frac{\sqrt{kTC}}{q} \]  

(2.12)

where \( k \) is Boltzmann's constant and \( T \) is the absolute temperature. This noise arises from the uncertainty in establishing a potential¹⁴,¹⁵ across the pixel/rail gap but is practically insignificant since the pixel/rail capacitance is just a few hundredths of a pF. Such is not the case with active matrix arrays which have pixel capacitances of about a pF.

Free charge is created by the quantum action of light photons just below the photoconductor interface in the presence of a non-zero electric field. If the photogeneration efficiency \( \eta \) were unity and the number of photons matched the number of charges to be switched there would be an uncertainty in switched charges \( N_A \) associated with the Poisson statistics of the optical photons \( \phi_{op} \) given by:

\[ N_A = \sqrt{\phi_{op}\eta} = \sqrt{\phi x} \]  

(2.13)

with the value of \( g \) generally greater than 100 (20 keV/(50eVx4)). Since the ratio \( N_A/N_\phi = \sqrt{g} = 10 \) this source of noise is insignificant with respect to x-ray noise unless it arises in a manner where it is not correlated to x-ray noise, eg. if a voltage bias were to be applied during readout.
Fig. 2.15(a): PAS pixel (100 x 100 μm) readout noise components with no bias applied to the readout rails. $N_x$ is the x-ray quantum noise, $N_Q$ is the shot noise of the charge read out, $N_A$ is the amplifier noise (shown assuming a 20 cm long rail), $N_{kTC}$ is the thermal reset noise; $N_R$ is the sum of all the noise sources except for $N_x$ and is given for rails 20 and 50 cm long. $N_x$ exceeds $N_R$ for exposures greater than 1 μR.

Fig. 2.15(b): Same as for Fig. 15(a) except that a 1 Volt readout bias is applied to the readout rails. Bias noise associated with $N_Q$ causes $N_R$ to compete with $N_x$ at exposures of a few μR.
We calculate and plot in Fig. 2.15(a) the noise sources identified above. The x-ray exposure range was taken as 1 μR to 1000 μR; \( W_a = 50 \) eV and the a-Se layer 300 μm thick (quantum efficiency of 66% calculated with the aid of Eq. (2.6)). The capacitance of the pixel was taken to be 0.035 pF which gives an \( N_{\text{TC}} \) of 75 q, smaller than all other fixed noise sources. The total readout noise, \( N_r = N_{\text{a}} + N_{\text{q}} + N_{\text{TC}} \) and is calculated for detector lengths of 20 and 50 cm. In Fig. 2.15(b) the same calculations are performed except with an additional readout bias of 1 volt applied, which ensures that the maximum readout time for any exposure level is \( \approx 1 \) μs; see Fig. 2.10. Fig. 2.15(b) also shows how the addition of this bias compromises quantum limited performance at exposure levels below \( \approx 1 \) μR.

2.7 Discussion

2.7.1 Readout time

If one were to use the two rail geometry (as an approximation) and assume that the capacitance of the PAS pixel-rail gap pixel is given by the approximate formula \( C = \varepsilon_{\text{se}} (d_p)^2 / d_g \) (Fig. 2.9), then the mean electric field \( E_{\text{PAS}} \) across the gap would be \( Q / [\varepsilon_{\text{se}} (d_p)^2] \) where \( Q \) is the charge stored on the pixel and \( (d_p)^2 \) is the area of a pixel. Note that \( E_{\text{PAS}} \) is independent of \( d_g \), thus the transit time of charge is proportional to \( d_g \). In the PID approach the capacitance of a pixel is given by the parallel plate formula \( C = \varepsilon_{\text{se}} (d_p)^2 / d_{\text{se}} \) where \( d_{\text{se}} \) is the thickness of the PID a-Se layer. The electric field in the a-Se layer of the PID arrangement is given by \( E_{\text{PID}} = Q / [\varepsilon_{\text{se}} (d_p)^2] \) and hence the transit time of charge is proportional to \( d_{\text{se}} \). Thus based upon these assumptions the ratio of the PAS to PID readout times would be \( d_g / d_{\text{se}} \), a small number (as desired) since \( d_g \ll d_{\text{se}} \). In fact as the readout rail pixel gap (\( d_p \)) of the PAS approach is made small the capacitance of the junction increases more slowly than \( 1 / d_g \) (Fig. 2.9) which has the fortunate consequence of reducing PAS
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Readout time more than the ratio $d_{se}/d_g$. Capacitance calculations show that for $d_{se} = 500 \, \mu m$ and $d_g = 5 \, \mu m$ the reduction in transit time is approximately 1000 rather than 100 ($d_{se}/d_g$). Thus the goal of reducing readout time by reducing the distance the charge carriers must move has been successfully achieved.

It is desirable to achieve a large readout signal in order to achieve a high signal to noise ratio (SNR). Thus we consider the effect on readout time of injecting increasing amounts of charge into the readout gap and the additional effect of a decreasing potential on the signal pixel due to significant discharge.

For radiographic procedures where the smallest exposure is likely to be $> 100 \, \mu R$ the amount of charge on a pixel generates a large enough field (Fig. 2.13) such that readout time is small enough (Fig. 2.10) that a bias is not likely to be needed. Therefore we consider the pixel geometry of Fig. 2.14(c) where the electric field is due solely to the charge stored on the signal pixel. In Fig. 2.14(c) the signal current (curve A) for the pixel geometry is shown where $F \sim 1/20$. In this case space-charge does not impact the field in the gap and the pixel potential does not decrease significantly. In this situation the current (hole) is concluded after 8 $\mu$s which is just the transit time of holes across the junction with a constant field of 1.8 V $\mu m^{-1}$.

However for the maximal signal case when $\Lambda_p = 1/4$ the fraction of charge injected (F) into the junction is $\sim 1/2$ the charge stored on the pixel. Curve B of Fig. 2.14(c) represents this case. Surprisingly the hole current reaches a maximum sooner than for the small space-charge case, but on the other hand it takes longer, about 40 $\mu$s, to terminate. We conclude that switching an amount of charge comparable to the charge stored on the pixel will increase the charge transfer time by about 4x over the case where space-charge effects and discharge are insignificant.

Therefore for radiographic procedures (taking 100 $\mu R$ to be the minimum detector exposure) we see that without space-charge effects the pixel readout time is $\sim 3 \, \mu s$ (Fig. 2.10).
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However due to the space-charge and discharge effects as discussed above, the pixel readout time will be increased by a factor of 4 to about 12 μs. The readout time for an array size of 4000x4000 (radiographic mode) would be 192 seconds when performed serially or if performed in parallel (1/2 line at a time) only 96 ms.

For fluoroscopic procedures the number of pixels read out is much less than in radiography. We will assume that fluoroscopic frame sizes are 512 x 512 pixels. In spite of this low number of pixels, the fluoroscopic charge signal is so low (due to the low exposure rate per frame) that it probably would be necessary to apply a small bias to achieve a frame readout time of 1/30 sec. Working backwards from the data of Fig. 2.10 we will assume that a bias of 0.1 Volts will be necessary with a minimum pixel read time of ~ 10 μs. From Fig. 2.14(a) we see that space-charge effects with a constant potential across the gap increase signal readout time by about 2. If half a line of pixels can be read out at once the frame readout time is then 512 x 2 x (10 x 2) μs = 20 ms. This time is smaller than 1/30 sec and hence fluoroscopic readout is possible if the noise is low enough as discussed in the next section.

2.7.1 Noise

With a readout bias of 1 V quantum noise limited operation can be maintained from 2 μR to detector saturation (~ 1000 mR) since as shown in Fig. 2.15(b) quantum noise (N_q) exceeds readout noise (N_r) down to exposures of about 2 μR, even for detector lengths of 50 cm (Fig. 2.15(b)). For fluoroscopic systems the situation can be improved by reducing the readout bias so long as the frame readout time is maintained below 1/30 sec. As discussed above a 0.1 V bias should provide a short enough frame readout time for a fluoroscopic system (512x512 pixels). At a 0.1 V bias readout noise becomes comparable to quantum noise at about 1 μR which is acceptable for fluoroscopy. These low readout noise levels should be practically attainable since
the PAS readout is not encumbered with the "injection" of charges \( Q=CV \) that are associated with voltage operated switches i.e. FET switching devices that apply an appreciable switching voltage \((-5 \text{ V})\) over a switch capacitance of about 1 pF.

### 2.7.2 Dynamic range

We have previously noted the slower than linear increase in pixel rail capacitance as \( d_g \) is decreased. This has the consequence of developing high fields in the readout gap even for relatively small x-ray exposures when \( d_g \) is small. Thus with \( d_g = 5 \mu \text{m} \) breakdown field strengths \((-100 \text{ V } \mu \text{m}^{-1})\) at exposure levels of \(-350 \text{ mR}\) are reached as shown in Fig. 2.13 and hence the dynamic range of the PAS approach is reduced somewhat below that of PID methods, (shown to exceed 1000 mR). However this level of exposure is unlikely to be required except for mammography. Also the PAS system starts to become non-linear at exposures above approximately 50 mR. This relatively early departure from linearity is due mainly to the drop in the DCE(X), shown in Fig. 2.11, which occurs as the electric field starts to bend away from the pixel electrode as signal charge is accumulated.

### 2.7.3 Resolution

The highest spatial frequency of interest in medical imaging is \(< 20 \text{ lp/mm}\) and up to this spatial frequency the MTF of an a-Se layer is \( > 50\% \) at all clinical beam energies\(^3\). The resolution of the PAS method is therefore dictated primarily by the sampling pitch of the system. However the presence of signal on one pixel electrode could possibly disturb the potential on neighbouring pixels i.e. inducing cross-talk and thus reduce resolution. This effect was examined by putting a signal charge on a pixel, obtaining the field solution, and then comparing the potential developed on the charged pixel with the potentials developed on the uncharged pixels. From this simulation
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we found this effect to be about 15% to direct pixel neighbours diminishing to 5% or less for indirect neighbours. Thus the MTF at the highest frequency, as determined by the sampling pitch, will only be reduced by about 15% by cross-talk.

In the model the pixels have been treated as part of an infinite strip. The resolution discussed above pertains to the direction orthogonal to the readout strips. In the direction parallel to the readout strips the resolution could suffer more cross-talk effects if there were no interpixel shielding septa. We assume however that such septa as shown in Fig. 2.16(a) would be present in a real device and have widths comparable to the rail width and also be connected to the rails. Therefore pixel cross-talk effects in the direction of parallel to the readout rails would be similar to those in the orthogonal direction.

2.7.4 Doubling readout speed

The possibility of using double readout rails as shown in Fig.2.16(b) to shield neighbouring PASs from each other so that they could be all read out simultaneously rather than alternately was considered. It was found, however, that the shielding afforded by the narrow double rails was only fair and also reduced the signal.

2.7.5 Practical considerations

The analysis in this chapter does not consider any of the practical problems which would be encountered with making PAS electrode structures. As discussed in chapter 4 two main points will have to be addressed: obtaining blocking contacts and the effects of surface traps. Without good blocking contacts charge leakage from the pixel and rail structures can be expected and would have to be controlled by choosing the appropriate electrode materials, with attention to polarity and geometric details eg. reducing edge fields to control leakage. The effects of trapping
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Fig. 2.16(a): Top view of a PAS system with inter-pixel septa in the x direction to prevent cross-talk and resolution loss in the z direction. The readout rails are along the z direction.

Fig. 2.16(b): Inserting two sets of rails in the pixel rail gaps allows the possibility of reading out an entire line of pixels simultaneously. The idea is to have field lines from a pixel couple only with the rails immediately adjacent to it. The readout rails are therefore no longer shared and the readout of one pixel would not affect (ideally) its neighbour.
states at the a-Se/glass interface is to prevent ballistic readout as assumed in this chapter. The effects of trapping states on surface photoconductivity are discussed in detail in chapter 3 and their implications for the PAS readout method are analyzed and discussed in chapter 4.

2.8 Summary and conclusion

It has been shown that a simple photoconductively activated switching (PAS) device is, in theory, possible through either the radiographic, fluoroscopic, or in some other as yet unspecified electrode biasing arrangement. Through such suitable biasing arrangements it is possible to sensitize the a-Se with a strong vertical field during the x-ray exposure and collect signal charges on pixels located at the interface of the a-Se and transparent dielectric. The vertical field also ensures that the resolution of the readout method is dictated primarily by the sampling pitch of the system. After the x-ray exposure the presence of the signal charges on the pixels creates a local lateral field to readout rails, which are also at the a-Se/dielectric interface and in very close proximity to the pixels. The readout rails are held near a virtual ground potential by virtue of their connection to low noise charge sensitive amplifiers. A PAS switching element consists of a central pixel surrounded by a readout rail on each side with photoconductive material separating the pixel and rails. During a PAS readout operation, light is shone on one of the pixel-rail gaps generating free electron hole pairs which allow for a net transfer of charge from the pixel to the readout rail (discharge). For a signal to develop on the readout rails during the photoconductive discharge process it is essential that the pixel charge be shared with a passive capacitive element i.e. the rail not undergoing photoconductive discharge.

In the radiographic mode of operation the voltage on the bias electrode of the a-Se layer is positive and the bias voltage on the dielectric layer is negative, creating a unidirectional vertical electric field from the bottom of the a-Se to the top of the transparent dielectric layer. For readout
the x-ray bias is turned off to remove the vertical field in the pixel-rail gap and allow a purely lateral field (proportional to the signal charge on the pixel) to develop in the pixel-rail gap. A small readout bias of 1 Volt applied to the readout rails will insure a pixel readout time of about 1 μs even for exposures as small as 1 μR. The extra readout noise contributed by this relatively small bias is smaller than x-ray quantum noise down to about 1 μR. This quantum limited exposure is more than 100 times smaller than that achievable with PID readout methods.

In the fluoroscopic mode of operation the x-ray bias voltages on the a-Se and dielectric layers are both positive, creating vertical fields of opposite directions in the a-Se and transparent dielectric layers. This removes the vertical field component in the pixel-rail gap, a hindrance for readout operations, but introduces a strong lateral field unrelated to x-ray exposure. The lateral field is removed by scanning the system prior to a sequence of fluoroscopic images. The "dummy" scanning negatively charges the pixel electrodes so that their potential becomes nearly the same as the readout rails. During x-ray exposure positive signal charge is brought to the pixels which reduces their negatively charged state and causes a lateral field to redevelop in the pixel-rail gap. During a readout scan the pixels are "recharged"; the readout signal being proportional to the amount of recharging required.

To conclude we note that the long readout times and bias noise problems of PID approaches have been reduced by more than 100 in the PAS approach by photoconductively moving signal charges a short distance of ~ 5 μm near the photoconductor surface rather than ~ 500 μm through the photoconductor bulk. Readout times and bias noise of the PAS approach are predicted to be small enough that x-ray quantum noise limited readout at fluoroscopic exposure rates is a possibility. Resolution of the system is dictated principally by the pixel sampling pitch, the dynamic range of the system is ~ 10^4 with the system response becoming non-linear above approximately 50 mR (80 kVp beam). The simplicity of the device structure should make it
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possible to construct devices large enough for most radiological procedures at reasonable cost. The detector and scanner could be an integrated system or the detector could be similar to a screen-film cassette which is taken to a laser scanner for image readout.

Appendix 2.1

Before proceeding to set up a more elaborate set of matrix equations to solve the pixel geometry we discuss the nature of potential functions due to infinite length line and sheet charges and a method of dealing with the potential at infinity (in directions orthogonal to the axis of infinite extent of the lines and sheets). Note that the potential at infinity is an implicit boundary condition.

Using Gauss’ law it can be shown that the electric field $E$ due to an infinitely long line of charge is given by:

$$E(r) = \frac{\lambda}{2\pi \varepsilon r}$$  \hspace{1cm} (2.14)

where $\lambda$ is the line charge density, $\varepsilon$ is the permittivity of the medium, $r$ is the radial distance from the line charge and $\mathbf{l}_r$ is the unit radial vector. Whereas our problem formulation is in terms of scalar potentials we derive the potential by integrating the field with respect to a reference point:

$$\Phi(r) - \Phi(r_{ref}) = \int_{r_{ref}}^{r} E \, dr = -\frac{\lambda}{2\pi \varepsilon} \log_e \left( \frac{r}{r_{ref}} \right)$$  \hspace{1cm} (2.15)

It is often the case that $r_{ref}$ is taken to be at infinity, as for example with point sources, and the potential at infinity is taken to be zero or "ground". For point sources:
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\[ \Phi(r) - \Phi(r_{ref}) = \int_{r_{ref}}^{r} \frac{Q}{\epsilon} \frac{dr}{r^2} = \frac{Q}{\epsilon} \left( \frac{1}{r} - \frac{1}{r_{ref}} \right) \]  \hspace{1cm} (2.16)

from which it is clear that as \( r_{ref} \) is made very large the term \( 1/r_{ref} \) vanishes and the potential is finite (for \( r > 0 \)).

However with line sources the potential at infinity diverges logarithmically hence one might in this case choose to make \( r_{ref} \) large but only finitely so and define the potential at this large \( r_{ref} \) as ground. The problem with using a large \( r_{ref} \) is the introduction of a large constant which can introduce problems with numerical accuracy. In the solution of the parallel plate capacitor discussed in section 2.6.1 (Charge simulation modelling) if one ignores \( r_{ref} \) altogether the solution will be correct under some circumstances but incorrect under others. If for instance the potential of the "anode" electrode is set at \(+V/2\) and the "cathode" electrode at \(-V/2\) the solution as outlined is correct. If instead the electrode potentials are set at \(+V\) and 0 (the potential difference between the plates is still \( V \)) the solution will be slightly in error. The potentials of the electrodes at every point (on the electrodes) will be correct but away from the electrodes there will be a slight asymmetry of the potential as though a charge at a large distance (above the anode) were acting. Furthermore a check of the sum of the charges on both plates will show a slight positive excess. If one invokes a large \( r_{ref} \) as mentioned previously the solution approaches the symmetry expected and charge neutrality.

Based on these observations it was decided the best approach was to make the net charge of the model system zero necessitating that there always be at least one "ground" electrode at a reference potential different from other electrodes or space-charge in the system. However the requirement of charge neutrality introduces an additional equation to the matrix of
equations and may cause the system to be over constrained. To avoid this problem an integration constant $\Phi_{\text{ref}}$, which is often non-zero and unknown a priori, is introduced into the solution process. It is found that the system charge neutrality condition causes the potential calculated at infinity to approach the finite value $\Phi_{\text{ref}}$.

We now proceed to discuss other aspects of the line and sheet source functions. Using Eq. (2.15) one can determine the potential due to a sheet of charge by performing an analytic integration along the width of the sheet. With the centre of the strip (width $a$) located at $R$ and the observation point at $r$, the potential is given formally by:

$$
\Phi(r) = G(a, r-R) \sigma
$$

(2.17)

where $\sigma$ is the uniform surface charge density of the strip. The actual analytic form of the function $G$ will depend upon coordinate system conventions and orientation of the charge strip. In Cartesian coordinates for a strip lying along the x-axis and centred at the x-y origin the potential is given\(^9\) by:

$$
\Phi(x, y) = \frac{\sigma}{2\pi \varepsilon} \left\{ \log \sqrt{(x-a/2)^2 + y^2} - \log \sqrt{(x+a/2)^2 + y^2} + \frac{y}{y + \tan \left( \frac{x-a/2}{y} \right) - y \tan \left( \frac{x+a/2}{y} \right) + a} \right\}
$$

(2.18)

Space-charge in the implementation of CSIM is treated as lines of charge which can move under the action of the electric field as illustrated in Fig. 2.17. The potential of the lines is treated as:

$$
\Phi(r) = L(r-R) \lambda
$$

(2.19)
Fig. 2.17: CSIM modelling for the pixel geometry: electrodes are divided into linear strips of fixed or variable width (x direction) of infinite extent into the +/- z direction, space charge is represented as lines of charge and can move dynamically. The potential at say the ith electrode strip, location $R_i$, is calculated as the sum of potentials due to charge on all the other strips, its own self potential, and the contributions from the space-charge. Shown in the diagram is the vector $|R_i - R_j|$ which is used to calculate the potential contribution of the jth strip at the ith strip according to an equation similar to Eq. 2.5.
where \( L(r-R) = -\log_e(\frac{|r-R|}{2\pi\varepsilon}) \) with the line located at \( R \) and the observation point at \( r \). The integration constant associated with equations (2.17),(2.19) is dealt with as discussed previously. Note that the location and amount of line space-charge is a known quantity, generated under the action of light or x-rays in the presence of a field generated by charges on the electrodes.

Using the superposition principle we now proceed to set up a system of \( N \) linearly independent equations with \( N \) unknowns that determine what the charge distribution must be in order to maintain the electrodes at constant potentials. We divide the electrode structures into a total number of \( n \) segments of fixed or variable width (the segments do not all have to be the same length) and include space-charge as \( s \) lines of charge. As in section 2.6.1 the repeated index convention is used to indicate that a summation over the repeated index of a term is to be carried out. For the number of segments \( p \) whose fixed potentials \( V_i \) are known from boundary conditions the following equation applies:

\[
V_i - L_i \lambda_k = G_i j + \Theta_{nf}
\]

(2.20)

where \( i=1,...,p \), \( j=1,...,n \) and \( k = 1,...,s \). The left hand side of the equation is known whereas the constants \( \sigma_i \) and \( \Phi_{nf} \) are to be determined. For the \( m \) electrodes which are floating (the boundary condition on the electrode potential is unknown) the following equation applies:

\[
-L_i \lambda_k = G_i j + \Phi_{nf} - V_{f_i}
\]

(2.21)

where \( i=1,...,f \), \( j=1,...,n \), and \( k = 1,...,s \). For a given floating electrode the unknown potentials \( V_{f_i} \) are all the same (as are the \( V_i \) for the electrodes which have fixed potentials). The left hand sides of the equations (2.21) are set to a definite value \((-L_i \lambda_k)\) in order to consistently have the left hand side of the equation set a known value to be compatible with matrix solution methods used later.
Each electrode segment has a potential contribution from itself and all the other electrode segments so there are a total of \( n^2 \) terms in the first summations \((G_{i\sigma})\) of the right hand side of Eqs. (2.19) and (2.21). The entire system has a zero net charge, expressed in Eq. (2.22):

\[
-\lambda_k = \sigma \beta_i
\]  

(2.22)

where \( i=1,...,n \) and \( k=1,...,s \) which permits the calculation of the unknown variable \( \Phi_{\text{ref}} \). The introduction of \( \lambda_k \) is simply a construction to maintain the repeated index summation convention.

For the floating electrode structures there are corresponding equations, of the form given in Eq. (2.23), concerning their net charge \( xchg_j \), which may be non-zero due to the accumulation of an x-ray signal or photogenerated charge:

\[
\sigma \beta_i = xchg_j
\]

(2.23)

where \( j=1,...,m \) and \( i=1,...,f'(m) \) where \( m \) is the number of floating electrodes and \( f'(m) \) is the total number of electrode segments on the \( m^{th} \) floating electrode. The existence of equations (2.23) completes the linear set of equations and permits the determination of \( V_{f_i} \), the unknown floating electrode potentials on the right hand side of Eq. (2.21). In table 2.1 are summarized the range of the various indices used in the above equations.
TABLE 2.1

<table>
<thead>
<tr>
<th>N</th>
<th># variables to solve for</th>
</tr>
</thead>
<tbody>
<tr>
<td>p</td>
<td># fixed potential electrode segments</td>
</tr>
<tr>
<td>f</td>
<td># floating electrode segments</td>
</tr>
<tr>
<td>f(m)</td>
<td># electrode segments on the m&lt;sup&gt;n&lt;/sup&gt; floating electrode</td>
</tr>
<tr>
<td>n=p+f</td>
<td># total electrode segments</td>
</tr>
<tr>
<td>m</td>
<td># floating electrodes</td>
</tr>
<tr>
<td>s</td>
<td># space-charge lines</td>
</tr>
</tbody>
</table>

Finally one arrives at a matrix equation with the form:

\[ B = G \cdot X \]  \hspace{2cm} (2.24)

where \( G \) is a known "potential source" square matrix of \( N^2 \) elements, \( B \) is a known boundary vector of \( N \) elements and \( X \) is an unknown vector, length \( N \). The matrix equation (2.24) is shown in Fig. 2.18 with some of the elements filled out and categorized. The number of unknowns, \( N \), is given by:

\[ N = n + m + 1 \]  \hspace{2cm} (2.25)

where the additional unknown is due to the determination of \( \Phi_{\text{ref}} \). The solution of these equations was carried out by performing standard LU (lower and upper) triangular decomposition and iterative improvement techniques as outlined by Press et al.\(^6\). When Eq. (2.24) has been solved
Fig. 2.18: The matrix equation used to solve the pixel geometry. The boundary vector includes known quantities: voltages, space-charge, electrode charges and the net system charge. The source matrix contains potential source functions and binary valued terms to link the system of equations. The unknown vector is comprised of the charge densities on the strips, the floating electrode voltages and lastly the reference potential.
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capacitances can be directly calculated since the solution contains the charge densities on the electrode structures. The electric field was found by taking the negative gradient of the potential using a second order centred difference approximation.

References


Photoconductively activated switched (PAS) readout of a-Se
Chapter 3

Experimental and theoretical studies of charge transfer at an a-Se glass interface
3.1 Introduction

The photoconductive properties of amorphous selenium (a-Se) have been extensively studied by many researchers largely due to its relevance in the area of photocopying and x-ray imaging. The work of Pai and Enck\(^1\) introduced in chapter 1, and henceforth referred to as Pai and Enck, shows that an Onsager model of field assisted thermal dissociation can fully explain photogeneration in a-Se. Due to our interest in constructing a digital radiographic device (chapter 2) which would transfer charge laterally near the surface of a thick (300 µm) a-Se photoconductive film we have performed measurements to characterize charge transfer at an a-Se glass interface. We use the terms surface and interface interchangeably.

The primary purpose of our measurements was to determine how a narrow line of photogenerated electrons and holes actually move when experiencing the local lateral field in the gap between two surface strip electrodes that face each other edge to edge (Fig. 3.1). The charges are created with a brief (compared to transit times of carriers across the junction), pulsed line of light in the gap at the interface between a photoconductor and a transparent dielectric. We call the new experimental measurements surface time of flight (STOF) by analogy to the classic bulk time of flight (BTOF). In this experiment (a variant of which is shown in Fig. 1.8) a flash of light generates a sheet of carriers (either electrons or holes depending upon the direction of the electric field) which then moves through a photoconductor due to the electric field caused by a large surface charge or a bias voltage applied across the parallel conducting plates. The BTOF, a powerful tool for characterizing carrier properties in semiconductors and photoconductors, was first carried out by Haynes and Shockley\(^2\) and is usually referred to simply as TOF. It is called TOF because it is normally expected that all the carriers will move with a common velocity in the spatially constant electric field \(E\) and hence all will arrive at the collecting electrode at one time.
Fig. 3.1: Sample with a-Se deposited on a glass substrate with strips of chromium electrodes. The current is measured between two adjacent strips held at different potentials. The left strip is connected to a voltage source while the right strip is connected to a current amplifier which maintains it at virtual ground. The total current measured by the amplifier is due to a dark leakage current and a current due to photogeneration of carriers by the action of light shining on the gap between the rails.
Surface photoconductivity of a-Se from which their time of flight is directly measured. This behaviour is due to the fact that they suffer little trapping or dispersion and hence from a macroscopic point of view move ballistically with a velocity $v = \mu E$ where $\mu$ is the mobility of the carrier. Our STOF arrangement differs from BTOF arrangements in that the electric field is not constant across the gap and additionally that one must consider the movement of two carrier types (which are generated as initially overlapping collinear lines) rather than the movement of a single sign charge sheet. Working in the spirit of the BTOF ideas we calculated and plotted [Fig. 2.14(a),(b),c] in chapter 2 the expected currents that carriers would generate without surface trapping, dispersion or other unanticipated effects. However we found that the a-Se/glass STOF experimental currents were much smaller than expected from the above mentioned calculations and that the current profiles also differed radically from the expected.

In chapter 3 two principal things are accomplished: (1) the experimental techniques used to measure photoconductivity at the interface a-Se and glass are presented and the results thus obtained are given and discussed, (2) a new theory of surface photoconductivity for a-Se is developed to account for our unexpected results. The surface photoconductivity theory is based upon the postulate that a dense monomolecular layer of traps exists at the surface. With regards to (1), measurements of the bulk electron and hole mobilities of the samples were also carried out to verify that the samples indeed had nominal bulk mobilities whereas the STOF experimental results were quite different from expectations. The surface photoconductivity or STOF measurements were performed with both short light pulses (shorter than $\tau_p$, the transit time of the more mobile holes across the full width of the gap) and with much longer pulses. The fraction of the gap illuminated was typically ~ 16% (partial gap), but experiments with full 100% illumination (full gap) were also carried out. The short pulses elucidate the effects of fast trapping at the
Surface photoconductivity of a-Se

surface while the longer pulses performed with partial gap illumination demonstrate the effects of a space-charge buildup at the surface.

The objective of (2) is to show that it is possible to explain all observed lateral photoconductivity effects solely in terms of the effects of one new postulate: the existence of deep surface trapping sites. Otherwise we assume that the bulk electron and hole mobilities of a-Se obtained through bulk time of flight measurements apply to electrons and holes immediately below the surface and at all depths. Surface photoconduction in a-Se is explained by supposing that the electron and hole pairs generated in the exponential attenuation of light in a-Se thermally diffuse to the surface where they are trapped. The shallow penetration depth (0.05 μm) of blue light into a-Se allows rapid diffusion of carriers to the trapping surface causing a substantial reduction of the photoconductive signal. The photoconductive signal during the initial phase of a long stimulating partial gap light pulse (>> τ_p) reaches a maximum and subsequently declines to a much lower equilibrium value. This phenomenon is explained in the models by the buildup of space-charge trapped at the surface which collapses the electric field in the illumination region and chokes the current. However a single mono-atomic layer of surface trapping states just falls short of completely explaining all details of the experimentally observed photoconductive signals, suggesting that trapping states may extend a short distance into the photoabsorption layer.

3.2 Experimental materials and methods

3.2.1 a-Se strip samples

Our test samples, shown schematically in Fig. 3.1, consisted of a glass substrate 1.1mm thick with chrome strip electrodes 254 μm wide, ~500 nm thick and 1 cm long. Gaps between the strips ranged from 10.2 μm to 254 μm wide. A layer of chlorinated a-Se:0.35% As 300 μm thick was deposited on top of the electrode strip structure and lastly the surface of the a-Se had a 400 nm
uniform layer of indium, to serve as a bias electrode. Both the a-Se and indium were deposited thermally in a vacuum.

3.2.2 Optical apparatus

An optical apparatus, illustrated in Fig. 3.2, projected a laser beam ~40 μm wide and 1 cm long onto the a-Se surface in the gaps between the electrode strips. The light source was a 7 mW CW 442 nm (2.8 eV) Helium Cadmium laser which produced a circularly symmetric beam with a Gaussian intensity profile. The laser beam could be pulsed by an acousto-optic modulator (AOM) with an extinction ratio of 1000. The 1 mm diameter beam from the laser was passed through an 8x beam expander and focused into a narrow line onto the sample by a plano-convex cylindrical lens with a focal length of 15 cm.

From a visual inspection of the line its width was estimated to be ~ 40 μm. The width was estimated by comparison of the apparent line-width to the known width of electrode structures. We did not quantitatively measure the intensity profile of the line illumination. However an estimate of the lower limit of the width of the line can be found from Fraunhofer diffraction theory. For a parallel beam focused on a screen by a lens the first dark ring of an Airy disk for a circular aperture occurs at a radius \( r \sim 1.22 (f\lambda/D) \) where \( f \) is the focal length of the lens and \( D \) is the aperture diameter. A similar estimate is given for Gaussian beam optics in reference 4. For \( f = 15 \text{ cm}, \lambda = 0.5 \text{ μm}, \) and if \( D \) is considered to be the diameter of the entrance beam (8 mm), one calculates the beam diameter at the focus to be 23 μm.

Visual inspection was used to facilitate positioning of the beam on the sample. To prevent possible eye injuries from "direct observation" of the sample it was observed "indirectly" using a
Fig. 3.2: Optical arrangement used to project and pulse a narrow line of light in the gap between electrodes on the sample. An acousto-optic modulator (AOM) chops the laser beam.
large working distance microscope equipped with a CCD camera and TV monitor.

The sample was mounted on an X-translation stage and additionally the beam could be repositioned in the sample X-Y directions by tilting the laser beam steering mirrors. All beam positioning was accomplished manually. The sample was electrically shielded by grounded copper sheet above and below the sample. The top sheet was perforated in order to allow the pulsed light onto the sample.

3.2.3 Current preamplifier and associated electronics

One strip electrode was connected to a 10 MHz bandwidth DC coupled current preamplifier to measure photoinduced currents. The opposing electrode on the other side of the gap was connected to an adjustable high voltage power supply. The other sample electrodes were grounded. The large area bottom a-Se electrode was normally left floating. However to measure bulk photoconductivity properties of the sample it had an applied potential from an adjustable high voltage power supply.

The current preamplifier was a modified Canberra 2004 charge preamplifier. The first stage FET 100 MΩ feedback resistor was replaced by a 1 MΩ resistor and the integrating capacitor was removed. Additionally a post-processing pole-zero compensation capacitor was removed. The signal input connection to the preamplifier was directly coupled to the first stage of the preamplifier except when a 1 MΩ resistor was inserted for current calibration purposes. The response of the amplifier was calibrated by feeding a voltage pulse (50 mV 2 μs) to the preamplifier with the 1 MΩ input calibration resistor in place. The rise time of the preamplifier was found to be ~ 100 ns. The preamplifier's sensitivity was 2.2 nA/mV and its peak to peak noise was a few mV, depending slightly on the sample configuration. The preamplifier output was amplified by a NIM amplifier module and the output was connected to a 100 MHz digital oscilloscope which
Surface photoconductivity of a-Se was interfaced to a personal computer (PC).

A variable duration and repetition rate pulse generator was used to switch the AOM on and off. The AOM had a 1.0 μs optical response delay from the leading/falling edge of the TTL pulse used to turn it on/off. Whereas the photoconductive channel could being stimulated in a repetitive controlled fashion, up to 32 photoconductive pulses were averaged to improve the signal/noise (S/N) of the measurements.

3.3 Experimental results

3.3.1 BTOF

We performed BTOF measurements on our samples to verify that they had nominal bulk properties (mobility, Schubweg). BTOF measurements of hole and electron mobilities were made using a sample arrangement as shown in Fig. 3.3. A bias of 5000 Volts was applied to the ITO electrode on the top glass surface producing a field strength of 1.7 V/μm in the a-Se layer. Light of power 170 μW was shone in a defocused circular spot, size of approximately 1 cm in diameter. Since the amount of charges generated by the pulse of light was only about 1/1000 the number of charges associated with the capacitance (Q=CV) of the illuminated spot, space-charge effects were not important. Prior to each measurement the bias was removed and the sample was exposed to light to remove any remaining surface charge. The pulsed signal measurements were made a few seconds after the application of the bias voltage. In order to quantitatively interpret the magnitude of the signal response it is necessary to consider the electrostatic coupling of the amplifier to the electrode structure as given in references. The amplifier coupling efficiency Λ is given by:
Fig. 3.3: Arrangement used to measure the bulk carrier transport properties of the samples. The region of the sample where no strip electrodes were present was used. An additional piece of glass with a transparent (ITO) electrode was put on top of the sample so that a vertical electric field could be generated in the a-Se layer.
where $d_g \epsilon_g$ are the glass thickness and dielectric constant and $d_{Se} \epsilon_{Se}$ are the corresponding parameters for the a-Se. The photogeneration efficiency $\eta$, of the light must be taken into account and an Onsager expression for $\eta$ (given by Eq. (1.2) of chapter 1 as adapted for a-Se by Pai and Enck) was used. For speedier calculation purposes Eq. (1.2) can be approximated (when $\lambda = 450$ nm) by $\eta = a' |E|^b$ where $a' = 4.9 \times 10^4$ and $b = 0.42$ for $0.5 \text{ V/\mu m} < E < 50 \text{ V/\mu m}$; for $E < 0.5 \text{ V/\mu m}$ $\eta = 0.14$ and for $E > 50 \text{ V/\mu m}$ $\eta = 1.0$. For the case at hand $\Lambda_\lambda$ and $\eta$ were 0.082 and 0.18 respectively.

Shown in Fig. 3.4(a) is a hole BTOF measurement made with the top ITO bias positive. The relatively short light pulse (1 $\mu$s) generates a sheet of charge which moves across the sample with a velocity $v = \mu E$. The constant part of the signal (which defines the hole transit time $\tau_p = 8 \pm 1 \mu$s) is the displacement current, detected by the amplifier connected to the indium substrate, when the charge is moving at a constant velocity through the bulk. The decaying part of the signal occurs as the charge sheet, broadened somewhat from its initial 1 $\mu$s width due to dispersion effects, reaches the indium electrode. The constant part of the signal was 20 mV x 2.2 nA mV$^{-1}$ = 44 $\pm$ 5 nA. The hole mobility $\mu_p$ is found to be $0.2 \pm 0.02$ cm$^2$/V·s$^{-1}$ as calculated from $\mu_p = d_{se}/(\tau_p E)$ which is in very good agreement with previously measured mobilities$^{7,8}$ in a-Se of 0.18 cm$^2$/Vs. Using $\Phi$, the incident number of photons, $j$, the measured current, and $\Lambda_\lambda$ one can calculate the optical photogeneration efficiency, $\eta = \tau_p j/(\Phi \eta \Lambda_\lambda)$. It was found to have the value...
Fig. 3.4(a): Hole BTOF measurement. The constant part of the signal occurs as the sheet traverses the thickness of the sample.

Fig. 3.4(b): Electron BTOF. The time for electrons to traverse the thickness of the a-Se film is greater than the bulk trapping time, causing the signal to decay. The mobility of the electrons can be determined from the initial peak response.
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0.13 ± 0.05, less than the value of 0.18 predicted by Eq. (1.2). More careful measurements of reflection losses at the selenium surface and glass interfaces (which reduce the measured value) in the experimental apparatus are required to determine if the value is in significant disagreement with Eq. (1.2).

Electron BTOF measurements shown in Fig. 3.4(b) were made by reversing the polarity of the bias and extending the duration of the light excitation pulse width to 10 μs to partially compensate for the reduced signal strength caused by the lower electron mobility. Since E was relatively weak (1.7 x 10⁶ V m⁻¹) and the sample thick d_se= 300 μm, the predicted electron transit time based on published μ_p can be expected to be about 300 μs. It should be noted that the bulk deep trapping times for electrons and holes are critically dependent upon impurities but for the a-Se we used are typically greater than 100 μs but less than 500 μs. Due to the fact that the electron transit time across the sample was comparable to the bulk trapping time of electrons, the electron transit signal was never constant as was the case with the hole signal but decayed to a fraction of its value during 300 μs. However since the 10 μs light excitation pulse is short compared to the electron trapping time the electron mobility can be calculated simply by taking the ratio of the measured peak current signal (just at the end of the light pulse) to that obtained during the hole measurements and dividing by 10, the increased amount of light used during the electron BTOF measurement. The effects of trapping, in particular at the surface, are considered in more detail in later sections. From Fig. 3.4(a) and 3.4(b) we thus obtain μ_n = μ_p/10 x (14 nA)/(45 nA) = 0.0062 ± 0.0006 which is in good agreement with the accepted value of 0.0063 cm²/Vs.

3.3.2 Dark current
The dark current was measured for electrode spacings of 20.3 and 254 μm and no significant
Fig. 3.5: Dark current measurements. The current increases as the fourth power of the average field in the gap.

- Average Gap Field V/μm
- Dark Current (nA)

Power law fit

Gap = 20.3 μm

Gap = 254 μm
difference was found for the two different electrode spacings when the current was normalized to the average field in the gaps. The results are shown in Fig. 3.5. It was found that the current increased as the fourth power of the applied field. It was noted that the dark current had an initially higher transient level for several seconds after the application of the bias when the field strength was greater than 5 V/µm for the 254 µm gap and when the field was greater than 3 V/µm for the 20.3 µm gap. The magnitude of the initial transient became more pronounced as the gap field was increased. The results in Fig. 3.5 are current measurements taken several seconds after the impression of a higher field. Since both electrodes are the same one cannot have a true blocking electrode system (an electrode asymmetry is required). However for practical purposes one may consider the electrodes to be blocking for fields less than 2 V/µm since the leakage current is small (compared to photocurrents).

To rule out the possibility that the dark currents were due to leakage in the glass substrate or elsewhere in the measuring system a potential 10x larger was applied to a duplicate electrode structure which did not have a-Se evaporated on it. No leakage current was observed.

3.3.3 Partial gap, short pulse surface time of flight (STOF) results
The STOF measurements presented here were performed using a 254 µm surface gap. The line of light used for excitation was typically shone in close proximity (centre of line to edge of electrode ~25 µm) to one of the electrodes so that the time of flight of created charge packets (moving across the gap hypothetically with bulk mobilities and without significant trapping) would be maximised and of several µs in duration so that it could be resolved from the 1 µs light excitation pulse. Results for other positions are also given. The light pulse was 1 µs in duration which was as short as possible consistent with obtaining a reasonable signal from the a-Se considering the 7 mW output power of the laser. Assuming η to be given by Eq. (1.2), the amount
Fig. 3.6: The intensity of the electric field in a 254 μm gap between two electrode strips of the same width. For idealized electrodes of zero thickness the field becomes infinitely strong at the edges of the electrodes. Also plotted is the Gaussian profile of the line illumination. The full widths of the electrodes are not shown.
of charge generated in the gap was calculated to be 1/1000 the capacitive charge of the gap, thus ensuring that space-charge would not alter the electric field in the gap. The electric field in the gap is not uniform and its theoretical profile is shown in Fig. 3.6 as calculated in chapter 2 (note that for ideal electrodes of zero thickness the electric field becomes infinite as one approaches the electrode edge). To a first approximation one can expect the current (as detected in one of the gap electrodes) due to a non-dispersive narrow line of charge moving across the gap to be proportional to the electric field at that location and hence the current would be like the plot of Fig. 2.8(a) with the x-axis now time and the y axis current.

The nominal or average electric field across the gap was varied an order of magnitude from 0.4 to 4 V/μm. The lower field was determined from the sensitivity of the amplifier and the upper was chosen in view of the higher dark current, although at fields above 4 V/μm high dark currents did not appear to perturb the photoconductive signal. At a field of 2.76 V/μm the full gap transit time of holes and electrons, assuming bulk mobilities, would be 5.2 and 150 µs respectively. Shown in Fig. 3.7(a) is the current profile for the weakest and strongest fields and for a polarity configuration which would require electrons to traverse the width of the gap. Fig. 3.7(b) shows the two current profiles plotted with their magnitudes normalized. This was an unexpected result since a packet of charge moving across the gap unfettered by trapping or other possible effects would take much longer to conclude at a weak field as compared to a higher field. Shown in Fig. 3.8 are the current profiles plotted for positive and negative potentials at equal field magnitudes. The signal intensity and shape (apart from the expected polarity reversal) appears independent of the sign of carriers moving across the gap.

The STOF signal varied linearly with the applied field and the illumination intensity which is shown in Fig. 3.9(a) and (b) respectively. The above STOF measurements were repeated for different positions of the light line in the gap and the magnitudes of the peak signal are plotted
Fig. 3.7(a): Surface time of flight (STOF) currents for experimental conditions requiring (in principle) the transit of the electrons (slower moving carriers) across the full width of the gap. The estimated transit time of electrons for the highest field is \( \sim 100 \mu s \). The signal starts decaying immediately after cessation of the light pulse and does not show a current signature representative of the free movement of carriers across the junction.

Fig. 3.7(b): The data of Fig. 3.7(a) have been normalized demonstrating that there is no detectable difference in the current profiles for the strong and weak fields. If carriers were able to move freely in the gap the profiles would be substantially different.
Fig. 3.8: STOF current profiles with opposite biasing polarities. If charges were free to move across the gap the current profiles would have been radically different as one would involve the faster holes, the other the slower moving electrons. Fig. 2.14(a) and Fig. 2.14(b) show the current profiles expected from the free movement of carriers.
Fig. 3.9(a): The signal intensity (square data points) as a function of the average electric field across the gap. The straight line is a linear fit to the data points. Since the signal is linearly dependent upon the number of carriers and the number of carriers generated is weakly non-linearly dependent upon the field strength (Onsager theory) there should be a departure from linearity as shown in the Onsager curve.

Fig. 3.9(b): Signal intensity (square data points) as a function of light intensity. The line is a linear fit. As discussed in section 3.5.4 a simple calculation would suggest that bimolecular recombination would have caused saturation of the response. The reason this does not happen is developed in the theory section.
Fig. 3.10: The peak signal from STOF measurements as a function of the position of the line of light in the gap (plotted points). Plotted as a full line is the convolution of the gap field with the Gaussian profile of the light.
in Fig. 3.10. Also plotted in Fig. 3.10 is a convolution of the calculated gap field with the Gaussian optical line profile. The magnitude of the convolution function has been normalized to the largest measured experimental signal.

3.3.4 Surface signals due to partial gap long pulse excitations

It was found that extending the light pulse beyond a few µs lead to a more complex behaviour. The light was pulsed in the centre of the gap at a few Hertz for these measurements; the slow repetition rate was used to allow for charge relaxation between pulses. The nominal gap field was 1.2 V/µm. For pulses of 40 µs duration the signal reached a peak value after about 10 µs and then started declining as shown in Fig. 3.11. For pulses of 4 ms duration, as shown in Fig. 3.12(a), it can be seen that the signal rapidly reaches a peak as with the shorter 40 µs, starts a decline and finally reaches an equilibrium value after about 1 ms. Another experiment was done with 4 ms pulses but this time the sample also was continuously illuminated over the whole gap with a weak incandescent light source. The resulting behaviour is shown in Fig. 3.12(b) and it can be seen that the post peak equilibrium current level is about 1/3 more than without the incandescent lamp.

If the pulse repetition rate was increased from a few Hz to 70 Hz (without incandescent light) the current waveform shown in Fig. 3.13(a) was realized where it can be seen that the large initial peak observed at the slower repetition rate is suppressed. However if the sample is also illuminated with the continuous incandescent light at the higher repetition rate the sharp peak in the current returns as can be seen in Fig. 3.13(b).

3.3.5 Signals due to pulsed, uniform gap illumination

The effect of pulse illuminating the entire gap was explored. Shown in Fig. 3.14(a) is the response
Fig. 3.11: When the light pulse using partial gap illumination is extended in time a new type of behaviour emerges, the signal saturates and then starts to decline.
Partial gap illumination

Fig. 3.12(a): Partial gap illumination, 4 ms length pulses; pulse repetition rate a few Hertz.

Partial gap, pulsed illumination

Fig. 3.12(b): Pulsed (4 ms) partial gap illumination with continuous full gap diffuse light.
Fig. 3.13(a): Long (4 ms) pulses with a repetition rate of ~ 70 Hz. The signal maximum is less and does not show an initial peak value as with the slower repetition rate.

Fig. 3.13(b): Long (4 ms) pulses with a repetition rate of ~ 70 Hz. Continuous full gap diffuse light restores initial signal maximum and increases signal magnitude.
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to a 40 μs pulse. Compared to the line illumination as illustrated in Fig. 3.11 one can see that the signal continues to rise during the pulse length and the final achieved signal is larger (46%). The response to a 650 μs pulse is shown in Fig. 3.14(b) where it can be seen that an equilibrium is being established at the end of the illumination period.

3.3.6 Summary of key experimental results

Shown in Fig. 3.15 (with the narrow line of illumination near the right hand electrode) is a conceptual summary of key experimental results and comparisons to theoretical expectations as calculated in chapter 2. Fig. 3.15 (a) and (c) are results for the polarity which would cause the more mobile holes to traverse the gap. As depicted in Fig. 3.15(a) we expected the hole signal to continue long after the short illumination pulse (1 μs) and even increase later in time as the hole packet approached the negative electrode where the fields get strong. The measured overall signal in fact was much weaker than that predicted based on the relative high mobility of holes and the signal started a sharp decline immediately at the end of the light pulse. On the other hand in Fig. 3.15(b), with the polarity reversed, the measured signal strength due to the short illumination pulse was, discounting the expected initial burst of current due to holes as shown in Fig. 2.14(b), approximately that expected from carriers with a mobility similar to electrons. However again unexpectedly the current started a decline immediately upon cessation of the light pulse. In Fig. 3.15(c) and (d) the situations for long illumination periods (100 μs) are illustrated. Experimentally the signal did continue to increase for a period of time after the start of the long pulses, as expected due to the continued creation of carriers, but reached a peak value and then started a decline. In all the experimental results the signal magnitude was roughly that which would be expected if the carriers had an "electron-like" mobility (see section 3.5.2). The key question is: how can all of the above be explained in view of the fact that both electrons and
Fig. 3.14(a): Uniform full gap illumination with a 40 μs pulse. The signal does not saturate and decline as occurs for partial gap illumination as shown in Fig. 3.11.

Fig. 3.14(b): Uniform full gap illumination with a 640 μs pulse. The signal current due to light reaches an equilibrium value close to the end of the light pulse.
Fig. 3.15: Simplified summary of experimental current pulses compared to the expected currents. Fig. 3.15(a) and (b) are for short light pulses while 3.15(c) and (d) are for long pulses. The current is consistent with a carrier mobility near that of electrons but trapping or recombination is occurring which squelches the signal.
holes are being created? It is clear that trapping or recombination of some sort is occurring but how? In the next sections the physical picture and numerical model to naturally explain the surface phenomenon is developed.

3.4 Theory and numerical model: introduction

Our theory to explain the experimental results develops in terms of two concepts: surface trapping and the diffusion of carriers to the surface. First we briefly discuss the effects of trapping and also show from the experimental data of short pulse STOF measurements, that the observed photocurrent is consistent with a mobility similar to that of electrons. Then we proceed to show how the diffusion of photogenerated electrons and holes just below an a-Se surface, populated with electron and hole traps, would rapidly trap holes leaving more electrons than holes for photoconduction. A simulated random walk of an electron and hole towards the surface filled with traps is shown in Fig. 3.16(a). At first we consider only vertical trapping effects and do not include lateral (horizontal) effects such as separation of electrons and holes due to the surface horizontal electric field and the subsequent space-charge buildup and localized weakening or strengthening of the surface field related to the partial illumination of the gap. These and other lateral effects are treated later by using the standard continuity equations of semiconductor physics and a simplified electrostatic model. It is implicitly understood in these simplified "no lateral effects" trapping models that carriers are moving laterally, but that horizontally charge distributions remain homogeneous and constant. The current is simply proportional to the number of carriers present and the static horizontal field. Thus to summarize the theory and modelling is developed in two stages: (1) consideration of trapping effects only and (2) trapping effects combined with lateral electric field effects and continuity equations. Three theoretical models of varying complexity are developed, each with and without lateral transport.
Fig. 3.16(a): Simulated random walk of two particles, an electron and a hole, after their photogeneration a short distance beneath the a-Se surface. The time, on average of reaching a distance L, increases as the square of L.
Although we believe surface trapping effects dominate the surface photoconductivity of a-Se the effect of bimolecular or Langevin recombination of electrons and holes is also considered in some detail at the end of the next section, since a simple calculation based upon carrier cross sections and densities suggests it could be quite important. However our experimental data do not support significant bimolecular recombination and why this is so is revealed in the numerical solution of the models about to be introduced.

3.5 Theory with no lateral effects

The simplest model assumes one time constant characterizes the hole trapping and another constant specifies the electron trapping. This is called the double-constant model. A second more accurate approach assumes the time to trapping at the surface is proportional to the square of the photogenerated carrier distance beneath the surface. This is called the square-law model. The square-law model overestimates the effects of trapping but is analytically tractable (without lateral effects) and can be numerically solved quickly when later coupled with the electric field and the lateral equations of continuity. The third and most exact treatment of surface trapping is to solve the vertical diffusion equation of carriers to the surface and is called the vertical-diffusion model. Shown in block form in Fig. 3.16(b) are the three types of models developed to understand the experimental data. The time scale of physical events ranges from tens of picoseconds (thermal diffusion time-scale of carriers photogenerated just below the surface) to the many milliseconds encountered in long light-pulse experiments. It is because eight orders of magnitude in time are encountered that different models of varying complexity are needed to compute results in a practical length of time.
Theoretical modelling

Horizontal Continuity Equations \rightarrow Electric Field Equations

Single time trapping constant for each carrier type

**Double-constant model**

Multiple time trapping constants for each carrier type from vertical carrier profile

**Square-law model**

Vertical diffusion equation for each carrier type

**Vertical-diffusion model**

Fig. 3.16(b): Block diagram of the three models (double-constant, square-law, vertical diffusion) used to understand the experimental phenomenon. The three models treat the effect of surface trapping (vertical movement to the surface) with increasing degrees of fidelity. The effect of the horizontal movement of carriers is treated by using continuity equations and the effects of the electric field; both are coupled. For simplicity the horizontal effects can be ignored when considering short pulse events.
3.5.1 Effect of carrier trapping on current signal

Trapping or recombination removes carriers from transport, occurs in the bulk or at the surface, and results in a smaller current than expected otherwise. Note that when the electric field $E$, is temporally and spatially constant, the current $J$ is simply proportional to $q\mu_e E/\int n(r,t)dr^3 + q\mu_h E/\int p(r,t)dr^3$, where the terms in square brackets are the integral sums of the electron and hole charges at time $t$ in the gap. In a-Se, trapping is understood to be a process whereby a carrier (electron or hole) becomes lodged, more or less permanently. The rate of trapping is dependent upon the number of carriers present and the trapping time constant $\tau_c$ ($c$ is the carrier type, $p$ or $n$), which itself is inversely proportional to the cross sections of the trapping site and carrier. It can normally be assumed that the percentage of trapping states occupied is small and hence the process is effectively monomolecular. In contrast, recombination in a-Se is a bimolecular process and is proportional to the concentrations of both the electrons and holes. If one considers trapping to be of primary importance, the differential equation describing the number of electrons present $n$, at any time can be expressed as:

$$dn = G \frac{dt}{\tau_{nt}}$$  \hspace{1cm} (3.2)

where $G$ is the photogeneration rate and $\tau_{nt}$ is the electron deep trapping time. A parallel equation exists for the number of holes $p$; $G$ is the same for electrons and holes. Assuming no carriers present at $t=0$ and that $G$ assumes a positive non-zero constant value for $t > 0$, Eq. (3.2) has the solution:
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\[ n = G \tau_m(1-e^{-t/\tau_m}) \]  

(3.3)

with a similar equation for the holes. If we make the assumption (which is lifted later) that the experimental current data of Fig. 3.7(b) is due solely to one carrier, the electrons, and that the loss of electrons occurs with one time constant, then one may estimate the electron deep trapping time \( \tau_m \), to be roughly 1 \( \mu s \). The total carrier generation time (light pulse) was 1.0 \( \mu s \) for STOF measurements and space-charge effects were nil (i.e. \( E \) is constant). Thus the current is simply proportional to \( E \) and \( n(t) \). Therefore when \( t \) equals 1.0 \( \mu s \) (the experimental pulse width), which also happens to equal \( \tau_m \), Eq. (3.3) indicates the current is \( G\tau_m(1-e^{-t}) \). If no trapping occurred, at the end of the pulse (length \( t \)) the signal would have been \( Gt \). Therefore trapping has reduced the signal at the end of the experimental pulse by only 0.632 .

3.5.2 Calculation of apparent mobility of surface photoconduction

As summarized in Fig. 3.15 we were unable to directly detect the expected presence of two different carrier types. Therefore one can, as a simplification, assume that the current is due apparently (or effectively) to a single carrier with an apparent mobility (or that both carrier signs appear to have the same mobility). The apparent mobility of carriers was calculated assuming that the number of photogenerated carriers is given by the Onsager expression of Eq. (1.2). A strip 40 \( \mu m \) wide (\( x \) direction) and 4 mm long, \( z_{exp}(z \ direction) \) was pulse illuminated (1 \( \mu s \)) with a laser power of 110 \( \mu W \). The field strength was 2 \( V/\mu m \) and the peak current was 44 nA. The equation for the current \( J \), can be expressed as:

\[ J = \frac{dQ}{dt} = z \frac{dx}{dt} a_x \]  

(3.4)
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where \( \sigma_z \) is the photogenerated surface charge density of electrons and holes (in reality we know both carrier signs must be created and equally) and \( x \) is the direction of positive charge movement. The value of \( |\sigma_z| \) is \( \approx 2.45 \times 10^5 \times 0.1/(4 \times 10^{-3} \times 40 \times 10^{-6}) = 2.45 \times 10^5 \text{Cm}^{-2} \). Finally Eq. (3.4) can be used to yield the apparent mobility of the charge carriers:

\[
\mu = \frac{v}{\frac{J}{E}} = \frac{J}{E z \sigma_z}
\]

which for the case at hand yields a mobility of \( \approx 2 \times 10^{-5} \text{cm}^2\text{V}^{-1}\text{s}^{-1} \), i.e. a number \( 1/3 \) the electron mobility in the bulk. However the factor of \( 1/(1-\varepsilon^3) \) calculated from Eq. (3.3) reduces the difference to just \( 1/2 \).

A consistent and plausible picture explaining the observed results might be to consider the holes deep trapped with a time \( \tau_{\text{pl}} \ll 1 \mu\text{s} \), such that their contribution to the current compared to electrons is greatly reduced from the ratio \( \mu_p/\mu_n = 28 \), and that the observed current signal is due in significant measure to electrons which are deep trapped with a longer trapping constant \( \tau_{\text{tr}} \approx 1 \mu\text{s} \). We now proceed to show how this situation arises naturally assuming only that the interface of the a-Se and glass are filled with a high density mono-atomic layer of hole \( \text{and} \) electron trapping states. The mobilities of electrons and holes below this mono-atomic layer are assumed to be the same as that measured in the bulk.

3.5.3 Random walk or diffusion to surface trapping states

As first pointed out by Tamm it is plausible from quantum mechanical considerations\(^9,10,11\) that interfaces would be filled with a high density of surface states. As discovered by Shockley, in the first unsuccessful attempts to build a field effect transistor, these states unfortunately can be very effective at trapping free carriers. We now proceed quantitatively to investigate how diffusion of
carriers just below the surface of a-Se to surface trapping states would affect the observed current signal in a-Se.

3.5.3.1 Square-law model without lateral effects

In the square-law model it is simply assumed that it will take a time \( \tau_{a} \), given by:

\[
\tau_{a} = \frac{L_{a}^{2}}{D}
\]  

(3.6)

for a photogenerated electron or hole to walk or diffuse a distance \( L_{a} \) to the a-Se surface and be trapped. The diffusion coefficient \( D \) is given by the Einstein relation:

\[
D = \frac{kT}{q\mu}.
\]  

(3.7)

We assume that the density of surface trapping states in combination with the cross section for trapping is such that a carrier reaching the surface will always be trapped. Light in a-Se is attenuated exponentially\(^{12,13}\) at distances \( y \) below the surface:

\[
l(y) = l(0)e^{-\alpha y}
\]  

(3.8)

where \( l(y) \) is the flux at \( y \), and the attenuation coefficient \( \alpha \), is \( 2.0 \times 10^{7} \) \([\text{m}^{-1}]\) for light of wavelength 442 nm. The exponential attenuation of light will generate a distribution of carrier trapping times by virtue of (3.6). A typical experimental value of \( l(0) \) was \( 1.5 \times 10^{21} \) photons \( \text{m}^{-2}\text{s}^{-1} \).

One can derive some simple analytic results from the square-law model by positing that (3.3) applies to all distributions of trapping times or equivalently at all depths in the a-Se layer.
First note that for an incident surface flux $I(0)$, and no trapping or recombination we require:

$$\int_{0}^{\infty} n(y)dy = k \int_{0}^{\infty} \exp(-\alpha y)dy = I(0)$$

which implies $k$ equals $\alpha$ and hence we may write for electrons:

$$n(y,\alpha,t)dy = \alpha I(0) \exp(-\alpha y) \frac{y^2}{D_n} (1 - \exp(-\frac{tD_n}{y^2}))dy$$

(3.10)

with a similar equation for holes. For $t$ much greater than $(y^2/D_n)$, when the carriers are in equilibrium, setting the derivative of (3.10) to zero reveals the maximum carrier density occurs at a depth $y_{max} = 2/\alpha$. For $t = y^2/D_n$ we have found an approximation for the position of the maximum carrier density:

$$y_{max} = \left(\frac{2tD_n}{\alpha}\right)^{1/3} = 3. (3.11)$$

We can also integrate (3.10) exactly for limits $y = 0, \infty$ at $t = \infty$ and we find the total number of carriers in the bulk is $2I(0)(\alpha^2D_n)$; for $t= y^2/D_n$ the integration must be carried out numerically.

### 3.5.3.2 Vertical diffusion model without lateral effects

In the square-law model the use of Eq. (3.6) does not take into account the Gaussian probability$^{14}$

$$p(L_{\alpha\tau_\alpha}) = (4\pi D_\tau) -1/2 \exp \left(-L_{\alpha\tau_\alpha}^2/4D_\tau\right)$$

of finding a particle from its starting position and the effects of the trapping interface are ignored, which is to say that (3.6) overestimates the number of carriers
trapped at the surface. These shortcomings are overcome in the vertical-diffusion approach where the surface is treated as an infinite sink of carriers such that none are assumed to exist there since from a current point of view they are trapped and immobile. The other surface is treated as very far away as compared to diffusion distances. Ignoring lateral effects the problem is then to solve, with the above boundary conditions, the time dependent diffusion equation in one spatial dimension with an exponential generating function. The equation for electrons is:

\[
\frac{\partial n(y,t)}{\partial t} = G \exp(-\alpha y) + D_n \frac{\partial^2 n(y,t)}{\partial y^2}
\] (3.12)

with the boundary conditions \(n(0,t)=0\) and \(n(\infty,t)=0\). A parallel equation exists for the holes.

In numerically solving (3.12) the need for very small time steps (\(-10^{-11}\) s) arises in solving the vertical diffusion equation near the surface (\(y \sim 0\)). As a faster approximation we have also solved the vertical diffusion equations for short pulse light excitations and ignored lateral transport features (by assuming an infinite illumination width along the lateral \(x\) direction) and simply calculated the current as proportional to the sum of \(n \mu_n + p \mu_p\) where \(n\) and \(p\) are the integrated number of electrons and holes from all depths. This is a fairly good approximation, since for short pulses the horizontal electric field is essentially constant when space-charge effects are small.

3.5.3.3 Double-constant model without lateral effects

Now that a physical basis for the relative trapping rates for electrons and holes has been established we proceed to calculate an effective \(\tau_{\text{e}}\) (assuming \(\tau_{\text{e}} = 1.0\) \(\mu\)s) which will subsequently be used in the double-constant model with and without lateral effects. Using Eq. (3.7) to determine \(D\), and Eq. (3.6) to determine the diffusion time to the surface traps, and
assuming a mean penetration distance $y_p$ of $1/\alpha$, one finds a trapping time of $5$ ns for holes and $0.15$ $\mu$s for electrons. If we take the observed deep trapping time of $1$ $\mu$s [see Fig. 3.7(a)] to be primarily due to electron deep surface trapping $\tau_{et}$, we can calculate an effective penetration depth using Eq. (3.6), to have the value of $\sim 0.13$ $\mu$m. Using this value for $L_{et}$ in Eq. (3.6) one finds a trapping time $\tau_{pt}$, for holes of $\sim 0.04$ $\mu$s. We then find as before, using Eq. (3.3) for $t = 1$ $\mu$s (the experimental STOF condition), that the hole current signal would be diminished by a factor of $25$ and the electron signal only by $1.6$. Since the hole mobility is $28$ times larger than the electron mobility one concludes that the contributions to current from electrons and holes would be comparable making these assumptions. We note in passing that the STOF decay curves of Fig. 3.7 have a long decay tail which are not in accord with a monomolecular exponential decay nor a bimolecular decay scheme; one can attribute the small persistent current to the small minority of carriers generated relatively far below the surface which have a long surface trapping time.

### 3.5.4 Thermal recombination

Up to this point we have been building a theory of surface photoconductivity based upon surface trapping. We now digress for a moment to consider the possible effects of thermal recombination. The bimolecular thermal recombination rate can be understood as:

$$R_{cn} \rho n = v_n \sigma_{cnp} \rho n$$

(3.13)

where $v_n$ is the thermal velocity $= \sqrt{3kT/m_c}$, $m_c$ is the mass of the carriers which is expected to be close to the mass of a free electron, and the carriers each have an effective cross section $\sigma_{cnp}$. According to the work of Haugen and Kasap the value of $R_{cn}$ in a-Se is correctly given by the Langevin equation:
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\[ R_c = \frac{q(\mu_p + \mu_n)}{\varepsilon_0 \varepsilon_r} \]  

(3.14)

where \( \varepsilon_r \) is the relative dielectric constant of the material. For a-Se, \( R_c = 5.35 \times 10^{-14} \) m\(^2\)s\(^{-1}\) and note that if one calculates \( \nu_m \) assuming \( m_c = m_e \), the electron mass, one finds \( \sigma_{np} = 8 \) Angstroms, a somewhat large value.

If we make the assumption that carrier trapping dominates recombination we can estimate the amount of recombination occurring for pulse durations \( > \tau_m \), the longest trapping time constant, and then see if the assumption is self-consistent. From Eq. (3.3) it is seen that for times \( > \tau_m \) the number of electrons is in equilibrium at the value \( G \tau_m \) and the holes will have long been at the equilibrium value \( G \tau_p \) since \( \tau_n >> \tau_p \). Then for \( t > \tau_m \) the rate of bimolecular recombination is:

\[ dn = R_c \ G^2 \tau_m \tau_p \ dt \]  

(3.15)

If we use the maximum experimental value of \( I(0) = 1.5 \times 10^{21} \) m\(^2\)s\(^{-1}\), with absorption considered to be uniform over a depth of 0.05 \( \mu \)m, then \( L = 3 \times 10^{-8} \) and if we use the additional assumption that \( \eta = 0.18 \), we find \( G = L \eta = 5.4 \times 10^{27} \) m\(^{-3}\)s\(^{-1}\). The rate of bimolecular recombination from (3.15) using \( \tau_n = 0.15 \) \( \mu \)s and \( \tau_p = 5 \) ns is found to be \( 1.17 \times 10^{27} \) m\(^{-3}\)s\(^{-1}\) comparable to \( G \) and surface trapping. However the values of \( \tau_m \) and \( \tau_p \) we have used are probably too short as discussed near the end of section 3.5.3.3. Thus we must examine bimolecular recombination more closely. Therefore we consider what would happen if only bimolecular recombination were occurring, in which case \( p = n \), or of the case with also surface trapping occurring where we can make the approximation that \( \gamma \), the ratio of holes to electrons, is \( \tau_p / \tau_n \):
which has the solution:

\[
\frac{dn}{dt} = G \left(1 - \frac{R_\infty n^2}{G} \right) dt
\]  

subject to the conditions \( n=0 \) at \( t=0 \) and that \( G \) is constant for \( t>0 \). This solution predicts the number of carriers to saturate at a time of \( \approx 0.5 \) \( \mu s \), as shown in Fig. 3.17(a). This was not observed experimentally. In Fig. 3.17(b) the number of carriers expected after a 1 \( \mu s \) pulse, calculated using (3.17), is shown as the illumination level is changed. Thus the expected response is in clear disagreement with the experimental result shown in Fig. 3.9(b). This will be shown to follow from the separation of electrons and holes [Eq. (3.11)] which substantially prevents recombination.

3.6 Theory and implementation of lateral effects for the double-constant, square-law, vertical-diffusion trapping models

We have ignored to this point the effects of the complexities of lateral carrier movement arising from the different electron/hole mobilities, concentration gradients, spatial inhomogeneities etc. These effects must be considered in order to quantitatively calculate the absolute current and study the effect of space-charge buildup, especially for long pulse excitations and different illumination configurations (partial or full gap). Space-charge effects result from the lateral separation of charges due to the electric field and their subsequent surface trapping.
Fig. 3.17(a): Number of carriers \((n, p)\) left after the start of illumination at time \(= 0\). Only bimolecular recombination effects are considered. The light flux rate corresponds to the maximum rate encountered in the experiments and it is assumed the carriers are generated uniformly throughout the penetration depth \(y_p\) of the light.

Fig. 3.17(b): Number of carriers \((n\) or \(p)\) present \(1 \mu s\) after the start of a light pulse which is varied in intensity \((x\)-axis\). The light flux level corresponding to the maximum intensity experimental conditions was \(3 \times 10^{28}\) carriers \(m^{-3}\).
There are also other phenomena of interest such as: detrapping, thermal recombination, lateral diffusion and the effect of the field dependent photogeneration efficiency, $\eta$. We chose to develop a model based upon the standard continuity equations of semiconductor physics\textsuperscript{15} and a simple electric field model. The simplified electrostatic model we have chosen to use is one dimensional along the lateral $x$-axis and can be visualized as equivalent to a parallel plate arrangement. It is recognized that this one dimensional electrostatic model does not have all the features of the two dimensional model of chapter 2, which would allow for instance the charge carriers to experience a vertical field to or away from the a-Se interface. However, as will be shown, this effect only becomes pronounced with the presence of a relatively large amount of space-charge in the gap. In summary we have chosen the one dimensional model because it allows for a simple implementation, embodies most of the relevant physics believed necessary to understand the essence of the experimental results, and computation time is kept manageable.

3.6.1 Electrostatic field implementation

Our simplified electrostatic model is depicted in Fig. 3.18(a) which shows ideal plate electrodes extending into $\pm \infty$ along the $y$ and $z$ axis directions and separated a distance $d_x$ along the $x$-axis. We consider the right hand planar cathode electrode to be at ground potential with the left anode electrode at the origin at a positive bias. We divide the region into a finite number ($n$) of vertical ($y$-axis direction) strips of width $dx$ which have a net space-charge density $\rho(x_n)$. It is because there is no variation in the model in the $y$ or $z$ directions that the electrostatic model is considered to be spatially one dimensional. In all of the trapping models: double-constant, square-law or vertical-diffusion, blue light (442 nm) is assumed to either shine at a uniform intensity throughout
Fig. 3.18(a): Parallel plate model used to approximate electric field effects in the gap. Instead of solving Poisson's equation to account for the presence of space-charge, the CSIM method is used to calculate the charge densities on the anode and cathode required to maintain the impressed potentials. This simple approach reduces computation time to manageable levels.
the cross-section (x-axis direction) of the gap, or with a Gaussian profile of width \( \sigma_x \) centred at a location \( x \) within the gap. In the \textit{square-law} and \textit{vertical-diffusion} models the exponential variation of light intensity in the vertical y-axis direction is accounted for (resulting in a distribution of trapping times) whereas in the \textit{double-constant} model an average light intensity is used.

In order to solve the electric field problem we adopt a very simple form of the charge simulation (CSIM) concept\(^1\) we used in chapter 2. Since the space-charge density will be known from the photogeneration rate and the continuity equations (next section), the field problem is solved if we can calculate the charge densities on the anode and cathode. We have two boundary conditions: 1) the known electrode potentials and 2) the system (electrodes and gap) is charge neutral. The electric field of a planar sheet\(^6\) is simply:

\[
E(x) = \frac{\sigma(x_n)}{2\varepsilon_{Se}}
\]

where \( \sigma(x_n) \) is the surface charge density of the \( n^{th} \) charge sheet or electrode. The field is positively directed (+) if the coordinate \( x \) is > \( x_n \) and conversely negatively (-) directed. From the above conditions we can deduce that the anode charge density is given by:

\[
\sigma_A = \frac{\varepsilon_{Se} V}{d_g} \sum_{\mu=1}^{N} \frac{P \Delta x}{2} - \frac{1}{2d_g} \sum_{\mu=1}^{N} \sum_{\mu'=1}^{N} \rho \Delta x \sum_{\mu'=1}^{N} \rho \Delta x \Delta x
\]

where \( N \) is the number of charge segments and \( d_g \) is the width of the channel. A similar expression exists for the cathode charge density. The electric field is given as the linear superposition of all the charge in the system ie.:
3.6.2 Continuity equations

There are two continuity equations, one each for holes and electrons. The hole density is given by \( p(x) \) and the positive-definite electron density \( n(x) \) is such that \( p(x) = p(x) - n(x) \). Following Sze\textsuperscript{15} we can write the hole equation as:

\[
\frac{\partial p}{\partial t} = -\mu_p \frac{\partial E}{\partial x} + \mu_p E \frac{\partial p}{\partial x} + D_p \frac{\partial^2 p}{\partial x^2} + \frac{p_t}{\tau_{pd}} - R_c p n + G(E) - \frac{p}{\tau_{pt}}
\]  

(3.21)

and similarly the electron equation as:

\[
\frac{\partial n}{\partial t} = \mu_n \frac{\partial E}{\partial x} + \mu_n E \frac{\partial n}{\partial x} + D_n \frac{\partial^2 n}{\partial x^2} + \frac{n_t}{\tau_{nd}} - R_c p n + G(E) - \frac{n}{\tau_{nt}}
\]  

(3.22)

where \( \tau_{pd}, \tau_{nd} \) are the hole and electron detrapping times; \( p_t, n_t \) are the density of filled hole and electron traps (we assume the number of trapping states to be unlimited, an issue addressed later); \( G \) is the photogeneration rate = \( L \eta \), \( L \) being an equivalent volume illumination rate; \( R_c \) is the bimolecular thermal recombination rate, also known as Langevin recombination.

The continuity Eqs. (3.21), (3.22) are one-dimensional but in the square-law and vertical-diffusion trapping models the last two terms are treated two dimensionally. This is discussed immediately after the next section, which deals with the numerical techniques used to solve the
equations. Finally we note that the current in the model was taken to be the sum of Maxwell's displacement current and the current due to electron and hole movement:

$$J = e_{se} \frac{\partial E}{\partial t} + q_n n E + q_p p E.$$  \hspace{1cm} (3.23)

The current according to Eq. (3.23) was calculated at two surface planes within the gap in order to get an improved averaged result and as a check that the sum of displacement and physical currents (i.e., the movement of charges) was a constant (within the bounds of numerical accuracy) even when the magnitudes of the two terms were quite different.

3.6.3 Numerical solution of continuity equations

The continuity equations (3.21),(3.22) were solved numerically in two different ways: 1) an implicit Crank Nicolson \(17,18\) (CN) technique and 2) a modified forward time centred space (FTCS) method. The FTCS was stabilized by the use of a Lax stabilization technique which was modified from that given in reference 18 by reducing the amount of "numerical diffusion" (not to be confused with the physical diffusion terms in the equations) to the minimum amount required to maintain solution stability. Such conditions were generally small enough to avoid unphysical results. In both models the time step \(\delta t\) was chosen small enough so that the distance travelled by the fastest carriers (holes) experiencing the highest electric field would travel 1/10 the width of a spatial element \(dx\). Another condition was that \(\delta t < \tau_p\) the fastest trapping time. Shown in Fig. 3.18(b),(c),(d) are illustrations of the three models. The number of lateral elements \(dx\) was taken to be 100 and in the square-law and vertical-diffusion models the number of subsurface \(dy\) elements was generally several hundred, depending upon the simulation time. Both solution methods gave the same results but the more complex CN method was unconditionally stable whereas our modified Lax
Fig. 3.18(b): Illustration of the double constant model, with lateral transport, which has one constant for hole trapping and the other for electron trapping. The laser beam is assumed to penetrate a distance $y_p$ and generate holes and electrons uniformly throughout this depth. The electric field is considered purely horizontal in the region $y_p \times d_g$ and for speed of calculation is modelled by a parallel plate. The fringing fields contribute a large capacitance not accounted for in this approximation which is handled by the introduction of a normalization factor $C_n$. The lateral transport is modelled by the continuity equations using finite methods (dx) and is solved numerically using a Crank-Nicolson scheme.
Fig. 3.18(c): Illustration of the square law model with lateral transport. The laser beam is attenuated exponentially generating many carriers near the surface and few below the surface. For blue light the 1/e penetration depth is about 0.05 microns. Once carriers are generated at a depth $y$, the time to trapping is considered proportional to the square of $y$. In addition to a horizontal grid ($dx$) used in solving the movement of carriers in the x direction there is a vertical grid ($dy$) used to maintain a profile of the net number of electrons and holes as a function of depth. Electric fields are handled as in the double constant model.
Fig. 3.18(d): Illustration of the vertical diffusion equation model, with lateral transport. As in the square law model the laser beam is attenuated exponentially generating many carriers near the surface and few below the surface. Now however separate diffusion equations in the vertical direction, one for holes and one for electrons, are used to determine the vertical profile of electrons and holes. The surface boundary condition is a perfect sink as is the bulk boundary condition. The location of the horizontal bulk boundary is set an order of magnitude deeper into the selenium layer than the exponential penetration depth of the light. Electric fields are handled as in the double constant model.
method sometimes exhibited periodic instabilities during long simulation times. The tri-diagonal matrices of the CN method were solved using a routine given in Press et al\textsuperscript{18} while Ames\textsuperscript{17} gives the Thomas algorithm for the same problem. Calculation times on an IBM\textsuperscript{1} AIX RISC 6000 computer were about 2.4 sec/\(\mu\)s for the double-constant model, 38 sec/\(\mu\)s for the square-law model and about 1 hour/\(\mu\)s for the vertical-diffusion model.

3.6.4 Implementation of Square-law and vertical-diffusion surface trapping profiles into the lateral continuity equations

In order to include into the lateral equations the effects of different surface trapping times resulting from the exponential absorption of light into the a-Se surface coupled with the relationship of Eq. (3.6), each discrete point \(x_i\) along the x-axis of the square-law model had a vector of discrete elements \(y_{ji}\) penetrating into the y-axis direction a fixed finite distance \(y_{max}\) typically taken to be 20 \(y_p\). The second to the last term of Eqs. (3.21),(3.22), the number of photogenerated carriers, was calculated at each time step \(\delta t\), at each depth \(y_{ji}\) using Eq. (3.8) and added to the previous value. The last term of the continuity Eqs., the number of carriers removed by a random walk to the surface, was calculated at each \(y_{ji}\) by Eq. (3.6) and subtracted. Detrapping was maintained with one fixed time constant 10 ms, since we believe at this time the traps to be deep relative to the time scale of the simulations. The implementation of the other terms (movement of carriers due to concentration gradients, electric field, lateral diffusion) in the continuity Eqs. (3.21),(3.22) were maintained one dimensional by treating the concentration of hole carriers (\(p\)) and electron carriers (\(n\)) as a one dimensional value, i.e. the sum of each depth location \(y_{ji}\).

3.7 Reduced dimension effects of the electrostatic field model

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3.7.1 Capacitance normalization to a rail geometry

The electrostatic model is a "parallel plate" and it assumes the key features of the current signals are due to the effects of spatially localized surface trapping and lateral carrier movement, rather than the effects of curved particle trajectories under the surface which might occur with the development of a significant amount of space-charge in the gap. We will use the term "space-charge" to mean both free and surface trapped charge in the gap. By "significant" space-charge we mean that it is comparable to the amount of charge present on the gap electrodes as calculated from \( Q = C_g V \), where \( C_g \) is the gap capacitance and \( V \) the potential maintained across the gap. The hallmark of significant space-charge is the deviation of the gap field away from its initial value before photoexcitation.

The capacitance of the electrostatic model must be "normalized" to match that of the true rail geometry such that the development of space-charge effects occur after an equivalent amount of illumination (or time) encountered experimentally. For a plate separation of 254 \( \mu \text{m} \) (the experimental conditions), the parallel plate capacitance for an area \( 1 \times y_p \text{ m}^2 \), which corresponds to the region of photo-activity, is \( 1.1 \times 10^{14} \text{ F} \) and which can be thought of as a capacitance of \( 1.1 \times 10^{14} \text{ F/m} \) in the model. The CSIM modelling\(^1\) of \( C_g \) for rails 254 \( \mu \text{m} \) wide and with a 254 \( \mu \text{m} \) gap is \( 8.7 \times 10^{11} \text{ F/m} \). Therefore, at first guess, we would expect it to take \( ~1 \times 10^4 \) as much photogenerated charge to introduce space-charge effects in the experimental situation as it does on the simulation model. This we call the capacitance normalization factor, \( C_n \). Later we demonstrate that the value of \( C_n \) is actually closer to the value of \( 10^3 \). The capacitance normalization is implemented by dividing the light intensity \( L \), used in the model by \( C_n \) and multiplying the current \( J \) calculated in the model by \( C_n \).

3.7.2 Recombination effects
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The requirement of reducing the light intensity by \( C_n \) in order to handle space-charge effects correctly in the model reduces recombination due to the bimolecular terms \( np \) of (3.13) to much less than would experimentally occur. This effect was compensated for by multiplying both \( n \) and \( p \) by \( C_n \), calculating the amount of recombination and dividing that result by \( C_n \) to retain consistency with the reduced light level.

3.7.3 Charge storage capability of surface states

We assume that the surface contains of the order of one trap site per interface atom. For a gap of 254 \( \mu \text{m} \) width per unit length \( (\text{m}^{-1}) \) this is equivalent to a storage capacity of \((2.54 \times 10^{-4} \text{m/1x10^{-10}m} \times 1 \text{m/1x10^{-10}m} \times 1 \times 10^{-5} \text{ C m}^{-1})\). The value of \( C_g \) for 300 Volts is \(-3 \times 10^{-9} \text{ Cm}^{-1}\). Therefore, based on the above assumption, the onset of significant space-charge gap field distortion occurs before \( 1/1000 \) of the postulated surface states are filled.

3.7.4 Horizontal geometric field effects

The field due to an infinite sheet of charge, Eq. (3.18), as used in the model, does not vary with distance. The field due to a line of charge varies inversely with the distance as given\(^{19} \) by:

\[
E(l) = \frac{\lambda}{2 \pi \varepsilon r} l_r
\]

where \( \lambda \) is the line charge density, \( \varepsilon \) is the permittivity of the material, \( r \) is the radial distance from the line charge and \( l_r \) is the unit radial vector. It has been shown in chapter 2 how a 2D model using line charges and sheet charges can be implemented. However if one considers the field profile between a dipole of line charges of separation \( S_g \), the field varies only by a factor of 1.3
over the central 50% of $S_2$ and by a factor of 2.8 over the central 90%. Therefore the uniform field of sheet charges in the electrostatic model is a reasonable approximation to the field between dipolar line charges as could be considered to be occurring in the experimental situation.

3.7.5 Vertical geometric field effects

The parallel plate field model does not admit a vertical y-axis component of the field that would affect movement of carriers towards or away from the surface. However one can calculate from the diffusion time of carriers to the surface the strength of a vertical field component needed to compete with diffusion. We have:

$$E_y = \frac{y_y}{\mu \tau_d} \frac{kT}{q}$$

which for $y_y = 0.05 \, \mu m$ is approximately 0.5 V/$\mu m$ (Note that Eq. (3.25) does not depend upon the carrier mobility).

In order to develop a vertical field of the magnitude given by Eq. (3.25) it would be necessary to accumulate a very large amount of polarized charge in the junction. For a thin layer of charge, such as exists at the a-Se interface after a period of illumination, the vertical field at the interface is given by an equation of the same form as (3.18) except that the field is in the y (vertical) direction. Thus the absolute value of the local vertical field just above or below the interface is $- \sigma(x)/(2\varepsilon_{se})$ where $\sigma(x) = \rho(x)\alpha$, the equivalent surface charge density at the gap position $x$. In the next section we shall show, using the resulting surface charge distribution after a long period of illumination, that the magnitude of a vertical field from this amount of charge is far smaller than the value given by Eq. (3.25). Thus the effects of surface space-charge in pushing or pulling charge to or from the surface are weak compared to diffusion effects.
3.8 Theoretical modelling results

The equivalent amount of light used in simulations to generate the following theoretical results corresponded to experimental conditions of: 110 μW (442 nm) and a potential across the gap of 508 Volts. Both the equivalent light intensity and the potential conformed with the experimental conditions of section 3.5.2.

3.8.1 Double-constant model short pulse results

Shown in Fig. 3.19(a) is a double-constant model STOF simulation using a 1 μs pulsed 40 μm width Gaussian beam in the centre of the 254 μm gap. The electron and hole trapping times were set to extremely large values compared to the transit time of carriers across the gap. The value of $C_n$ used was $10^4$. The current rises linearly during the duration of the pulse and then remains constant until the leading edge of the holes reaches the cathode. The smaller electron current continues for a longer time. The hole and electron currents remain constant during the transit across the gap because the field is uniform and has not been distorted by significant space-charge. The equivalent maximum (expected) no trapping experimental current would be $\sim 0.64 \text{ A m}^{-2} \times y_p (0.05 \text{ μm}) \times z_{\text{exp}} (4 \text{ mm}) \times C_n (1 \times 10^4) = 1.3 \text{ μA}$. This current is about 30x larger than observed experimentally.

Shown in Fig. 3.19(b) is the current profile calculated with the double-constant model with an electron trapping time of 1 μs and a hole trapping time 0.04 μs. The equivalent experimental signal is $0.37 \text{ A m}^{-2} \times y_p \times z_{\text{exp}} \times C_n (1 \times 10^3) = 74 \text{ nA}$. The measured experimental signal was 44 ± 20 nA, the large experimental uncertainty is due to the light intensity measurements made at the sample.

3.8.2 Square-law model short pulse results
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**Fig. 3.19(a):** STOF simulation (double-constant model) without surface trapping effects. The signal rises linearly during the 1.0 μs light pulse (starting at t=0) whereas no carriers are lost to trapping and space-charge effects are negligible. The 40 μm wide line of light shines in the centre of the 254 μm gap between the rail electrodes maintained at a potential difference of 508 V. The current is constant as the holes approach the cathode (the electric field in the gap is uniform) and then drops steeply as the Gaussian packet of holes reaches the cathode. The electron current is smaller and continues for a much longer time due to the lower mobility of electrons. The associated capacitance normalization $C_n$ factor for the simulation is $10^4$.

**Double-constant model**

- $\tau_p = 0.04 \mu$s
- $\tau_n = 1.0 \mu$s
- $C_n = 10^4$

**Fig. 3.19(b):** STOF simulation with trapping effects using the double-constant model. The trapping times are 1.0 and 0.04 μs for electrons and holes respectively. The conditions of light illumination are the same as in Fig. 19(a): 1.0 μs light pulse, 40 μm wide Gaussian line centred at the midpoint of the gap (127 μm); the potential across the gap was 508 V.
In Fig. 3.20 are shown modelling results with the square-law model. The 1/e penetration depth \( y_p \) of the light attenuation was 0.05 \( \mu m \). The square-law model calculates an equivalent experimental maximum signal of 15 nA as can be determined from the current profile of Fig. 3.20(a). The free electron and hole carrier densities as a function of gap position are shown in Fig. 3.20(b) at the end of the 1 \( \mu s \) light pulse. Fig. 3.20(c) shows the electron and hole densities as a function of the depth below the a-Se surface at the gap positions of maximum carrier densities [Fig. 3.20(b)], again at the end of the light pulse. From Eq. (3.11) the expected maximum electron density occurs at 0.12 \( \mu m \) and that of holes at 0.36 \( \mu m \) and are indicated by the crosses in Fig. 3.20(c). Fig. 3.20(d) shows for comparison purposes the experimental signal normalized (reduced by 2.7) and superimposed with the square-law model signal.

### 3.8.3 Vertical-diffusion model short pulse results

Fig. 3.21(a) shows the current resulting using vertical diffusion to determine the rate of surface trapping. The equivalent peak experimental signal is \( 5 \text{ Am}^{-2} \times y_p \times z_{exp} \times C_n(1 \times 10^5) = 100 \text{ nA} \) which is larger than the square-law model and experiment. Apparently a minority of photogenerated holes manage to diffuse somewhat into the bulk as shown in Fig. 3.21(b) where they are relatively long-lived resulting in a current component which can be seen to drop at around 4 \( \mu s \) as they reach the cathode. The results (normalized to experiment) for the vertical-diffusion model which does not include lateral transport effects are shown in Fig. 3.21(c) but an absolute determination of signal current is not possible.

### 3.8.4 Double-constant model long pulse results

For long pulses we wish to understand the experimental behaviour for two different situations: 1)
Square-law model

\( y_p = 0.05 \mu m \)

\( C_n = 10^3 \)

Fig. 3.20(a): Square-law STOF simulation current profile; same illumination and Voltage as in Fig. 19. There are no free parameters in this model. The current magnitude and shape follow directly from the physical assumptions of the model, namely the existence of surface traps.
Fig. 3.20(b): The lateral electron and hole densities as a function of gap position 0.5 μs after the light pulse ended in the square-law model (Fig. 3.20(a)). The centre of the illumination is midway (127 μm) in the gap. The electrons have not moved far from the illumination point but the few remaining holes have significantly moved towards the cathode at the right. The hole density has been multiplied by 300x to make it visible.

Fig. 3.20(c): The electron and hole densities (square-law model) as a function of depth below the surface 0.5 μs after the light pulse ended. The lateral gap position at which the carrier densities are vertically examined is 150 μm. The hole density has been multiplied by 100 x. The crosses mark the predictions of Eq. 3.12 of where the maximum electron and hole densities below the surface should be.
Fig. 3.20(d): Comparison of square-law model result with experiment. The model result is 2.7 smaller in magnitude than the experiment and does not show as persistent a current at longer times after cessation of the light pulse.
Vertical-diffusion model

\[ y_p = 0.05 \, \mu m \]
\[ C_n = 10^2 \]

Fig. 3.21(a): STOF simulation using the vertical-diffusion model. Same illumination conditions and applied potential as in the square-law and double-constant simulations of Figs. 19 and 20. A smaller value of \( C_n \) has been used related to numerical solution requirements; however even at this lower value of \( C_n \) space-charge effects are not important. The peak signal level is about twice the experimental value. Enough holes diffuse into the bulk to show their current signature as they reach the cathode. This was not observed experimentally. The square-law model under estimates the current at longer times, the vertical-diffusion model over estimates it.

Vertical-diffusion model

\[ \text{Time} = 1 \, \mu s \]
\[ C_n = 10^2 \]

Fig. 3.21(b): Electron and hole densities (vertical-diffusion model) below the surface just at the termination of the 1 \( \mu s \) light pulse. The distribution of holes is more smeared out and there are more holes deeper into the bulk than in the square-law model. The result is a larger and longer lasting signal.
Fig. 3.21(c): Comparison of STOF experiment with the vertical-diffusion model (when lateral transport effects are turned off). The maximum currents of experiment and theory have been normalized. The vertical-diffusion model overestimates the number of carriers which reach the bulk region as evidenced in the relatively high current after the cessation of the 1.0 μs light pulse.
localized line illumination in the gap and 2) full gap illumination. The key feature to be accounted for in 1) is the initial signal maximum which is followed by a decline and eventual equilibrium much less than the initial peak value. The situation for 2) is similar except that an initial signal peak does not occur and an equilibrium maximum value is attained with the passage of time that is larger than that which occurs in case 1). We believe the behaviour in 1) is due to the lateral separation and subsequent accumulation of electrons and holes into traps at the surface (they do not substantially recombine) creating a space-charge dipole field that weakens the field in the illumination region reducing photogeneration and current. This premise will be demonstrated using the double-constant model where the weakened field results in a diminishing current with time that approaches zero at an exponentially asymptotic rate. Experimentally the asymptotic value was non-zero, probably due to either: the presence of weak ambient light illuminating the entire gap; the effect of neutralizing dark current; the action of vertical fields; a dielectric relaxation process perhaps involving recombination of trapped electrons and holes; or a detrapping phenomenon.

In order to investigate model predictions for long illumination pulses (>> 1 μs) the double-constant model was used rather than the square-law or vertical-diffusion models because: it mimics, in a simple way, the fact that holes are trapped at a faster rate than electrons and as a result computation times are short. With long pulse excitations we expect a buildup of trapped surface charge comparable to \( C_gV \). From simulation results we have found that it takes approximately 10x as much light in the model to cause space-charge effects as expected considering the value of \( C_n = 10^4 \) derived from simple capacitance arguments. For the double-constant simulations we used electron and hole trapping times of 1.0 μs and 0.04 μs respectively; the electron and hole detrapping times were set at essentially an infinite length. The voltage across the gap was 300 Volts because this was the voltage used during the long pulse experiments. Fig. 3.22 shows simulation results for a 40 μs light pulse using different values of
Fig. 3.22: Long pulse (40 μs) and partial gap simulation using the double-constant model. Different values of the capacitance normalization factor $C_n$ have been tested to find the value which corresponds to experiment. When these curves are compared to the experimental result of Fig. 3.11 it is seen the value of $C_n = 10^3$ is approximately the correct value.
Fig. 3.23(a): Space-charge distribution (double-constant model) in the gap after the end of a 40 μs pulse; \( C_n = 10^3 \), 300 V across gap. For reference the illumination profile is shown. The regions of positive and negative trapped charge at the surface start to diminish the electric field strength in the localised region where the light shines (see Fig. 23(b)).

Fig. 3.23(b): Electric field in the gap at the end of a 40 μs pulse; double-constant model, conditions same as for Fig. 3.23(a).
Fig. 3.24(a): The current resulting from illuminating the centre part of the gap for 1 ms. The model used was double-constant, 40 μm Gaussian line illumination, $C_n = 10^3$, 300 V across gap. The current goes into decline due to a buildup of space-charge which collapses the field in the gap. Note for comparison the experimental result of Fig. 3.12(a).

Fig. 3.24(b): The electric field in the gap at the end of a 1 ms partial-gap illumination pulse; double-constant model, same conditions as for Fig. 3.24(a). The field has essentially collapsed in the centre of the gap reducing the current to nearly zero.
Fig. 3.24(c): The vertical electric field that would exist (at end of 1.0 ms light pulse) in the gap arising from a surface charge density taken as the sum of the volume charge density over the thickness of the illumination depth $y_p$; double-constant model, same conditions as for Fig. 3.24(a).

The vertical field was calculated assuming that it is directly proportional to the surface charge density. See section 3.7.5.
Fig. 3.25: The current resulting when the entire gap is uniformly illuminated; double-constant model, \( C_n = 10^3 \), 300 V across 254 \( \mu \)m gap. Light starts shining on gap at \( t=0 \) and stays on for 1 ms. The initial current rise is faster than the experimental result of Fig.3.14(b).
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C_n. When we compare these results to the experimental results of Fig. 3.11 we conclude that C_n = 10^3 corresponds to experimental observations.

In Fig. 3.23(a) is shown the space-charge distribution (essentially charge in surface traps) in the gap for the illumination level C_n = 10^3 after 40 μs of centre gap illumination. The illumination profile is shown for reference. Fig. 3.23(b) shows the gap electric field profile; the potential difference maintained across the gap was 300 Volts. Fig. 3.24(a) shows the current resulting when centre gap illumination is maintained for 1 ms. Fig. 3.24(b) shows the horizontal electric field in the gap while Fig. 3.24(c) shows what the vertical electric field would be assuming a volume charge density of thickness y_p compressed into an equivalent surface charge. The vertical field is taken as directly proportional to the surface charge density. Fig. 3.25 shows the current developed when the entire gap is uniformly illuminated for 1 ms with the integral light flux maintained the same as for the partial gap illumination.

3.9 Discussion

The fourth power law dependence of the dark current on the average gap field, was independent of the gap size (Fig. 3.5). The dark current presumably arises at the electrode edges, where the electric fields are greatest, and then follows a conduction path essentially in the bulk of the sample. This idea is consistent with the observation that the rather large dark currents did not alter the characteristics of the surface conduction phenomenon. As was first pointed out by Mott and Gurney^{20}, solid state space-charge limited currents (for a parallel plate geometry) should have a square law dependence of current upon applied voltage, assuming that at least one of the contacts is ohmic. This is a direct analogue of the Child-Langmuir 3/2 power law voltage dependence of currents in a vacuum diode. Yet Smith and Rose^{21} observed dark currents in single crystals of cadmium sulphide with a behaviour very similar to our a-Se dark current
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observations, that is with a much higher power law dependence. Although Rose\textsuperscript{22} developed an explanation for the CdSe behaviour, it is dubious that this explanation would also apply to a-Se. We suggest that the high power law dependence of dark current on voltage in our a-Se samples may be due to the way space-charge limits currents generated at the edges or points (imperfections) of the electrodes rather than a current arising uniformly (spatially) over the planar electrode structure in accordance to barrier theories.

Carrier mobilities and lifetimes in a-Se are sensitive to substrate deposition temperatures and dopants such as arsenic and chlorine. The bulk carrier properties we measured in our samples were well within the norm used for radiography and bulk carrier anomalies could not have been responsible for the small transient surface photoconductivity.

The short pulse (1 $\mu$s) \textit{double-constant} model signals of Fig. 3.8 made with fields an order of magnitude different showed no shape difference when normalized. This is direct evidence that carrier lifetimes are so short they do not travel significantly far in the gap and generate time of flight signatures of current indicating their arrival at the anode or cathode, as in BTOF measurements. The signal current is simply proportional to the electric field at the site of photoexcitation and decays as the carriers trap at the surface before they travel any appreciable distance. In Fig. 3.11 the STOF signal is shown to be greatest near the edges of the electrodes, qualitatively consistent with the electric field strength profile as shown in Fig. 3.7. Within experimental error Fig. 3.10(a) shows the photocurrent to be linear with the applied electric field. The Pai and Enck photogeneration efficiency of Eq. (1.2) predicts a weak field dependence of photocurrent upon the range of electric fields encountered in the experimental data plotted in Fig. 3.10. The absence of a non-linear signature may be due to lack of experimental sensitivity due to the noise introduced when the background temporally shifting dark current signal was subtracted to obtain the pure photocurrent.
The short pulse (1 μs) STOF or transient photoconductivity was, within experimental error, linear with light intensity [Fig. 3.10(b)]. In retrospect this result was surprising since the use of the bimolecular recombination coefficient, as determined by Haugen and Kasap\(^{23}\), in Eq. (3.13) predicts a sharp departure from linearity at the higher experimental intensity levels [Fig. 3.19(b)], if the carriers are assumed to exist at a uniform density throughout the photoexcitation layer of thickness \(\alpha\). The reason bimolecular recombination is not significant is due to the reduced carrier concentrations caused by surface trapping and the *vertical spatial separation* [Fig. 3.21(c), 3.22(b)] of the electrons and holes that results from their different diffusivities. The *square-law* and *vertical-diffusion* models which take into account the effects of vertical diffusion predict an insignificant amount of bimolecular thermal recombination.

The theoretical modelling of the 1.0 μs photoexcitation STOF is summarized in the semi-log plot of Fig. 3.26 with an experimental trace added for comparison. The no-trapping result clearly shows how much larger the signal would be without surface effects. This puts into perspective the effectiveness of surface trapping mechanisms, as realized in the other simulations, in reducing the signal. The simplified *square-law* model predicts a signal smaller than experiment due to its overestimation of surface trapping; however it demonstrates a decay tail in qualitative agreement with experiment. The *vertical-diffusion* model overestimates the signal magnitude due to the diffusion of a sufficient number of holes into the bulk and these same holes also generate a time of flight current signature as they reach the cathode. It is likely that if the *vertical-diffusion* model were to incorporate a thin film of trapping states a small distance (\(\leq \alpha\)) into the bulk, then the experimental results could be reproduced. The hypothetical currents resulting from longer wavelength light with deeper penetration depths are shown in Fig. 3.27 where it is assumed (unrealistically) that \(\eta\) is the same for all wavelengths.

The modelling results of long pulses shown in Fig. 3.25(a)(b) for both partial and full width
Fig. 3.26: Summary of results for 1 μs pulsed illumination (STOF) with 40 μm line illumination. The top curve illustrates the magnitude of the signal expected without trapping effects. The experimental signal was much smaller than this and the vertical-diffusion and square-law models bracket the experimental result.
Fig. 3.27: Hypothetical STOF signals (1 μs light pulse) which would arise if light penetrated to greater depths yet maintained the same photogeneration efficiency as blue light ($y_p=0.05 \mu m$).
gap illumination produce signals in agreement qualitatively and quantitatively with experimental results. With partial gap illumination the buildup of laterally separated space-charge, Fig. 3.24(a), reduces the local electric field that in turn reduces photogeneration and current \((j \propto E)\). When full gap illumination is modelled the current does not diminish with time since an appreciable space-charge can only develop very near the anode and cathode. In chapter 4 a simpler model is developed to explain the photocurrent due to full gap illumination. The non-zero current found experimentally for partial gap illumination is likely due to the space-charge nulling effects of dark current. The introduction of ancillary diffuse light throughout the full gap during narrow gap illumination [Fig. 3.13 (b)] illustrates the plausibility of this argument.

In the semiconductor literature surface effects are generally setup as a surface minority carrier recombination problem with the diffusion current at the surface equated to a surface recombination rate of minority carriers at the surface \(i.e.\) for an n-type material:

\[
qD_p \frac{\partial p(0,t)}{\partial y} = qS_r p(0,t)
\]  

(3.26)

where \(S_r\) is the surface recombination velocity. The recombination mechanisms are considered to be similar to those in the bulk, which for an indirect semiconductor such as crystalline Si (c-Si), are through intermediate recombination centres \(N_{brc}[m^{-3}]\), in the band-gap. However at the surface \(N_{arc}[m^{-3}]\) can be very large and have a dominant effect over bulk recombination. In n-type material for low-injection (the number of photogenerated carriers \(< n_m\), the majority carrier density) we can say:

\[
S_r = v_m \sigma_p N_{arc}
\]  

(3.27)

where \(v_m\) is the thermal velocity and \(\sigma_p\) is the effective cross section of the minority carrier. It is
assumed there are a large number of electrons present that can recombine with the hole once it has interacted with the recombination centre.

It is well known that a-Se can hold a surface charge and it is also well known that if carriers find themselves in the bulk of a-Se (via photo-injection or charge injection at a non-blocking contact) they move freely and can support a large current. This strongly suggests that the surface of a-Se is populated with a large number of deep traps. For this reason, and because the indirect effects of a large lateral buildup of surface charge were observed, we believe charge trapping, not recombination, is the correct physical way to view surface effects in a-Se. Ignoring lateral space-charge buildup effects (ie. reduced currents and photogeneration due to locally weakened fields) a surface recombination picture is mathematically equivalent to a trapping model where the density of surface traps is considered proportional to the $S_r$; an infinite $S_r$ equivalent to a 100% probability of a carrier being trapped at the surface; and a zero $S_r$ equivalent to no traps at the surface.

In passing we also note that a-Se is neither an n or p type semi-conductor, but rather a photoconductive insulator, and hence there is no low injection rate per se since $np = 0$. Therefore a physical picture of photoinjected surface recombination would have to involve the densities of both electrons and holes in Eq. (3.26). In fact, there would be two coupled recombination equations, substantially complicating the mathematics.

Nonetheless Enck has modelled surface effects in a-Se using an $S_r$ of 150 cm s$^{-1}$. Similarly we have solved the vertical diffusion Eq. (3.12) using the differential boundary condition of Eq. (3.26) in order to compare the trapping model with the surface recombination approach. The assumption of an $S_r$ of 150 cm s$^{-1}$ poorly matches the electron and hole distributions necessary to account for the low currents measured experimentally. An $S_r$ of at least 15000 cm s$^{-1}$, ie. essentially infinite, is required to account for the measured low currents.
Fig. 3.28(a): Electron sub-surface densities for surface recombination velocities, $S_r$ of 1.5 and 150 ms$^{-1}$. The results are similar to those of Fig. 3.21(b).
Fig. 3.28(b): The sub-surface density of holes for $S_r=1.5$ and 150 m/s. The density is much more sensitive to the $S_r$ than the electron density is. Only with the very high $S_r$ of 150 ms$^{-1}$ does the density drop enough to become comparable to the profile shown in Fig. 3.21(b).
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However, the surface recombination approach, which literally involves recombination of electrons and holes, cannot account for a buildup of space-charge, the later being responsible for our experimentally observed collapse of current (partial gap illumination) as shown in Fig. 3.13.

Shown in Fig. 3.28(a) and (b) are solutions of Eq. (3.12), for electrons and holes respectively, after an illumination time of 1.0 µs assuming two different S_r. The S_r of 150 cms\(^{-1}\) generates a profile of electrons similar to that required by the trapping model to account for the current contribution by electrons. However the case is different for holes, with too many holes present at the end of the illumination time. Not until a S_r 100 times greater is used does the number of holes diminish enough to account for the low observed photocurrent.

By calculating the minimum strength of a vertical field (acting over the diffusion time of carriers to the surface) required to sweep carriers from the surface and prevent trapping, we arrived at the field given by Eq. (3.25). This field agrees remarkably well with the field strength observed by Pai and Enck where the Onsager theory of Eq. (1.2) failed due to surface "recombination" (our interpretation is trapping). We tabulate in Table 3.1 estimates of α from the data of Hartke and Regensburger\(^2^5\) for the colours of light used by Pai and Enck in their η measurements. Knowledge of α then allows an estimate of the vertical field strength, using Eq. (3.25), where η would rapidly depart from the value predicted by Eq. (1.2). We reprint in Fig. 3.29 the measured and theoretical η curves determined by Pai and Enck and mark the field strengths where our trapping theory predicts η should plunge in value.

See Table 3.1 next page
3.10 Conclusion

Surface photoconductivity in a-Se is very low owing to the existence of deep electron and hole traps at the surface. Diffusion of photogenerated carriers to surface traps accounts qualitatively and quantitatively for the observed transient photoconductivity resulting from short pulses of illumination. The trapping model also accounts for the photoconductive signals obtained when the illumination is practically continuous and illuminates the electrode gap in part or in full. A physical model based upon the concept of surface recombination velocity, which is normally used to explain transient photoconductivity in semiconductors such as c-Si, does not apply to a-Se. A
Fig. 3.29: Measured and theoretical data for $\eta$ as given by Pai and Enck. Eq. 3.25 predicts that $\eta$ should depart from the theoretical expectations (the solid lines) at fields ranging between $6.8 \times 10^5$ and $1.5 \times 10^6$ for light between 400 and 600 nm respectively (see Table 3.1).
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simple use of the thermal recombination (Langevin) coefficient for a-Se would seem to suggest that bimolecular recombination would be important at the surface at the light intensities used in the experiments presented here. However this is shown not to be the case due to the separation of electrons and holes due to their different diffusivities.

It has long been known that the free surface of a-Se is very good at holding surface charges and the results presented here strongly indicate that this is due to a very thin layer of deep traps. That the resulting lateral surface photoconductivity in a-Se is poor is due to the fact that light with appreciable photogeneration efficiency is attenuated very close to the surface (0.05 μm) where it generates carriers that quickly diffuse to the surface and are trapped. A simple equation [Eq. (3.25)] has been derived which predicts the magnitude of a vertical field required to move carriers away from the surface of a-Se if an appreciable photocurrent is to be realised. The predictions of this equation agree approximately with the experimental data of Pai and Enck1.

The effects of surface traps on a practical device such as the type of PAS we have outlined in chapter 2 clearly indicate that the device would not operate as originally conceived unless traps were to be reduced by the use of a suitable interface layer. Similar efforts were required in order to make FETs made with c-Si useful. In chapter 4 we address in further detail the ramifications of trapping on PAS operation and show that for full gap illumination the presence of trapping causes surface photoconductivity to behave as a light dependent resistance.

Appendix 3.1

The following derivation for the bimolecular recombination (Langevin) coefficient in a-Se has been given by SO Kasap (private communication). Consider an electron hole pair and the motion of a hole with respect to that of an electron. Recombination occurs if the hole enters the capture
radius $r_c$ around the electron. Assume that the mean free path of the hole is much smaller than the capture radius. Thus the hole does not approach the electron with a thermal velocity $(1/2 m_e v_h^2 = 3/2 kT)$ but with an effective drift velocity due to the field of the electron:

$$v_{dh} = \mu_n E = \mu_n \left( \frac{q}{4\pi\varepsilon_0\varepsilon_f \varepsilon_r^2} \right)$$

The capture or recombination time $\tau$ is given by:

$$\tau = \frac{1}{S_c v_{rh}/n}$$

where $v_{rh}$ is the relative velocity of the hole with respect to the electron, $S_c$ is the capture cross section area $4\pi r_c$ and $n$ is the electron concentration. The hole is moving towards the electron with $v_{dh}$ and the electron towards the hole with $v_{de}$ so that:

$$v_{rh} = v_{dh} + v_{de} = (\mu_n + \mu_d)E = (\mu_n + \mu_d)\left( \frac{q}{4\pi\varepsilon_0\varepsilon_f \varepsilon_r^2} \right)$$

The capture occurs when the hole enters $r_c$ where $E = E(r_c)$ therefore:

$$\tau = \frac{1}{4\pi r_c^2 (\mu_n + \mu_d)\left( \frac{q}{4\pi\varepsilon_0\varepsilon_f \varepsilon_r^2} \right)n} = \frac{\varepsilon_0\varepsilon_r}{qn(\mu_n + \mu_d)}$$

Finally the rate of recombination is the rate at which holes are being captured ie:
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\[
\frac{dp}{dt} = \frac{p}{\tau} = -\frac{qpn(\mu_n+\mu_p)}{\epsilon_0\epsilon_r} = -pnR_e.
\]

References


Chapter 4

Summary and future work
4.1 Summary of motivation for the PAS approach

Investigation of the PAS method was motivated by a desire to overcome some shortcomings of PID readout methods previously investigated. In the PID methods the signal charge must be discharged through the entire thickness of the a-Se layer, which to maintain a high QE must be 500 μm for general radiography, leading to a relatively long pixel discharge time and hence total readout time. Additionally in the PID approach a large bias must be present during readout to keep discharge time less than the bulk trapping time, typically in the range of 100-500 µs for well prepared a-Se. Unfortunately the level of bias required generates a noise source which compromises PID performance at low exposure levels.

In chapter 2 it has been shown that a photoconductive surface readout method (PAS) of a-Se for digital radiography is possible which would overcome the readout and noise problems of PID approaches. Two readout scenarios were analyzed: (1) a radiographic method which turned on a high unidirectional vertical bias field throughout the entire PAS structure, but only during an x-ray exposure, (2) a fluoroscopic method which applied a bi-directional vertical bias field at all times during the operation of the device (including readout). The analysis assumed bulk carrier transport properties of a-Se. A key physical idea for the operation of the PAS readout method is reciprocal sharing of a pixel charge signal with two adjacent "readout rails". Readout light is shone in only one of the two pixel/rail junctions which allows development of a readout signal. This idea is a topological variation of the PID readout method. In the PID approach the pixel size was determined by the size of the readout beam, in the PAS approach the resolution is fixed by the pixel pitch width.

A very attractive practical feature of the PAS readout method is its simplicity, which should make it straightforward and economical to manufacture. It should be easy to make the device very
large since only one photolithographic layer is required and any defects which were to occur in manufacture would likely only compromise a few of the readout rails at most. Thus to manufacture a large device, as for instance 14"x17" in chest radiography, simply requires the ability to project a photolithographic pattern on a large glass sheet, etch the electrode pattern and finally evaporate the a-Se onto the glass in a large enough vacuum system. It is interesting to note that both the glass substrate and the a-Se detection layer of a PAS device are amorphous materials which can both be made in large uniform sheets.

Having established that PAS readout could work in principle, we suggest that chest radiography would be a good first application. Chest radiographs are large and an integrated system comprised of a fixed detector plate and laser scanner, which is most suitable for PAS readout, is not a disadvantage.

4.2 Possible noise advantage of PAS type readout over active matrix readout

There are two fundamental limiting noise sources in both phosphor and a-Se active matrix readout approaches: (1) the capacitance of the sensor line as the device is made large and (2) the kTC noise associated with the storage capacitors shown in Figs. 1.6 and 1.10 of chapter 1. The "storage" capacitance may be increased by design but it will always have a minimum value of about 1 pF associated with the intrinsic design requirements for proper operation of the TFT. The PAS approach suffers, as with active matrix approaches, from the readout rail capacitance noise but it has much less kTC noise because the capacitance of a pixel to a rail is only a few hundredths of a pF. The kTC noise associated with 1 pF is ~ 500 electrons whereas with careful charge amplifier design the amplifier noise associated with the capacitance of a rail line 20 cm long can be as low as 200 electrons.

When an active matrix TFT is switched (eg. typically with 5 V on the gate line), substantial
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charge signals ("charge-injection") are developed on the charge amplifier due to the capacitances of the TFT mentioned above (see Fig. 1.10 of Chapter 1). In principle the pulses are symmetrical with the rising and falling edges of the switching signal and should cancel. However, in reality, the subtraction is not perfect and since the injection signals are so large compared to the x-ray signal a residual signal noise, comparable to or larger than kTC or amplifier noise, it is difficult to completely suppress charge-injection effects. Also there will be other sources of cross-talk in an active matrix device, say from noise on the DC power supply (resulting from the transient currents required to switch the TFTs) operating the TFTs. This noise will couple to the analogue power supply for the charge preamplifiers compromising their performance. On the other hand with switching performed photonically, as with the PAS method, there are no charge-injection noise sources and minimum cross-talk or ground-loop effects. Thus, for yet another reason, the PAS readout approach has the potential of being a lower noise readout method than active matrix approaches. Unfortunately the lower noise readout is most important at low exposure fluoroscopic frame rates and since the PAS device is mechanically scanned, its lower noise advantage might be compromised by other practical problems. Nevertheless the low readout noise of PAS is important to note and perhaps could be used in a modified form of an active -> passive matrix readout. It is conceivable that one might use light to activate an array of phototransistors similar to the array of voltage activated transistors of an active matrix array.

4.3 Implications of surface trapping states for PAS readout

In chapter 3 the experimental results of surface photoconductivity at an a-Se/glass interface were given and the current was found to be less in magnitude and also qualitatively different from that calculated in chapter 2, which assumed known bulk properties of a-Se. The experimental results revealed that the surface photoconductivity decayed in approximately 1 μs (much shorter than the
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bulk trapping time of ~ 100 μs) and that the apparent mobility (for a 1 μs pulse) was similar to that of electrons, even in biasing arrangements which would have favoured the movement of the more mobile holes. The hypothesis was then put forward in chapter 3 that a high density of both electron and hole trapping states exist at the a-Se glass interface. Starting with this assumption, a theory and numerical model were developed which accounted for the wide range of experimental observations obtained. We now address the impact of surface trapping on the operation of PAS operation.

4.3.1 Pixel readout time with surface trapping

Without surface trapping effects, a minimum pixel readout time of 1 μs was found, in chapter 2, to be theoretically possible by: (1) maintaining a weak bias readout field (0.2 V μm⁻¹) across the readout gap and (2) shining a short pulse of readout light τᵣ just at the positive edge of the readout gap. The photogenerated holes then moved across the gap, while their counterpart, the slower moving electrons, were neutralised at the positive electrode. The duration of τᵣ is set << τᵣ, the transit time of holes across the gap. In this way the much more mobile holes would facilitate a faster charge transfer and a higher instantaneous current than if the electrons were to be used. The amount of charge which could participate in the charge transfer is "space-charge" limited at a value of 1/2 the charge stored on the pixel electrode, assuming the capacitances of the pixel to each of the two surrounding readout rails are the same. The Schubweg, or range of carriers, is defined by Sᵥ = μEτᵥ, where τᵥ is the carrier trapping time. In the bulk τᵥ is > 100 μs for well prepared a-Se. Thus at a field of 0.2 V μm⁻¹, Sᵥ for holes is > 360 μm and is large compared to the readout gap (~5 - 10 μm) so as not to be of consequence, so long as bulk trapping times are assumed.

An experimental result of chapter 3 indicated that the highest current could be obtained
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in a PAS arrangement (with surface trapping) by shining light in the full width of the pixel-rail junction instead of using partial gap illumination, where the idea was to use a biasing arrangement causing only the most mobile carriers, the holes, to move across the gap. However it was found with partial gap illumination that the channel can become "choked" by a local buildup of space-charge, opposing the applied field, as electrons and holes separate laterally and become trapped at the surface. For uniform full gap illumination the lateral buildup of space-charge is eliminated and from Fig. 3.14(b) we see that a sustainable current of ~ 30 nA is obtained under the conditions of 100 μW light illuminating a region 1 mm long and the full 254 μm electrode gap.

We now develop a simple physical model to calculate the maximum sustainable current using full gap illumination and will show that the gap acts resistively, unlike the bulk space-charge limited behaviour when trapping is not present. For lateral carrier movement near the a-Se surface, carriers are trapped with a relaxation time $\tau_{\text{rel}}$ given by $(y_p^2)/(kT\mu/q)$, where $y_p$ is the distance the carrier was created below the surface (0.05 μm for blue 442 nm light). Thus for instance at room temperature and at a field of 10 V μm$^{-1}$, the surface $S_b = \mu E \tau_{\text{rel}} = qE(y_p)^2/(kT)$ which is 1.0 μm for both electrons and holes. The fact that the surface $S_b$ for electrons and holes is the same allows us to view surface photoconductivity, caused by full gap illumination, in a simple way.

Shown in Fig. 4.1 is a diagram of the gap between the readout rail electrode on the left and the pixel electrode on the right (the electrodes are only shown in part). The thickness of the electrodes for convenience are assumed to be equal to the depth of penetration of the light $y_p$. The gap separation is denoted by $d_g$ and the width of the pixel is symbolized by $W$. Light of uniform intensity is shone on the entire gap with a total power of $I$. The total number of electrons $N_e$ and the number of holes $P_h$, generated in the gap are each given by:
Fig. 4.1: Model of the gap between a rail on the left and a pixel on the right. The electrodes are taken to be a thickness equal to the depth of penetration of the light into the a-Se layer. The gap has an area $d_g \times W$ which has a total power of $I$ shining uniformly on it.
where $h$ is Planck's constant, $v$ is the frequency of the light, and $\eta(E)$ is the Onsager photogeneration efficiency which depends upon $E$, the electric field strength in the gap. We assume that the field is uniform throughout the gap.

We assume the carriers are evenly distributed throughout the thickness of the channel gap $y_p$ (to simplify the math) and define a generation rate $G$ per unit volume as $G = N/(y_p W d_y)$ and likewise define $n = N/(y_p W d_y)$ and $p = P/(y_p W d_y)$ as the number of electrons and holes per unit volume respectively. The surface traps of the gap capture electrons and holes in the way described above such that on average the electrons and holes travel equal and opposite lateral distances before being trapped. Then referring to Fig. 4.1 we can think of the carriers as hopping laterally, undergoing trapping such that the electron and holes on average neutralize each other in the gap, and then being renewed by light photogeneration continue with another hop etc. Thus no lateral space-charge can build up in the gap. The electrons and holes contribute equally to the current since for every hole which arrives at the cathode an electron arrives at the anode (since electrons and holes move equal lateral distances before trapping).

Next we assume that $t$, the readout time, is greater than the trapping times $\tau_{\alpha}$ for both electrons and holes. Using eq. (3.3) the number of carriers present after the start of photogeneration is $G \tau_{\alpha}(1 - \exp(-t/\tau_{\alpha}))$. Therefore in this case $n = G \tau_{n\alpha}$ and $p = G \tau_{p\alpha}$ and note that $\tau_{n\alpha}/\tau_{p\alpha} = \mu_p/\mu_n$. The current (per unit area normal to the direction of current flow) is given by $J = n q \mu_n E + p q \mu_p E$. We then substitute for $n$ and $p$ and find:
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\[ J = G_{\tau} a q \mu_n E + G_{\tau} a q \mu_p E = \frac{2G}{kT} \frac{q^2}{E}. \]  \hspace{1cm} (4.2)

Therefore the current \( J_{\text{ini}} \) travelling across the gap to the electrodes is given by multiplying Eq. (4.2) by the plane with area \( W \gamma_p \) normal to the conduction direction and it follows that:

\[ J_{\text{ini}} = \frac{(2Nq)}{d_g} \gamma_p^2 \frac{q}{kT} E = \frac{(2/ \eta(E) q)}{\hbar} \frac{\gamma_p^2}{d_g kT} E. \]  \hspace{1cm} (4.3)

In chapter 3 the experimental current measured for full gap illumination was 30 nA when the illumination power \( I \) was 100 ± 50 µW, the wavelength of the light was 442 nm and from table 3.1 the penetration depth of the light \( (\gamma_p) \) is \( 1/(2.0 \times 10^7 \text{ m}^{-1}) = 0.05 \mu\text{m} \). The value of \( E \) across the 254 µm gap \( (d_g) \) was 1.2 V \( \mu\text{m}^{-1} \) and from the value of \( E \) it follows that \( \eta \) is 0.2 from Eq. (1.2). Using these values the current predicted by Eq. (4.3) is 6.7 nA, an underestimate of the measured current of 30 nA. The model leading to Eq. (4.3) simplifies the depth distribution of carriers into a single number \( (\gamma_p) \) and assumes a square law dependence of the trapping time, an underestimate of the trapping time (which decreases the current) for reasons mentioned in chapter 3. There it was suggested that when modelling trapping in this simple way (the double-constant model) one should use an effective penetration depth of the light which agreed with the observed photocurrent decay time. Taking that approach the effective penetration depth of the light was found to be 0.13 \( \mu\text{m} \). Using this value for \( \gamma_p \) the value of the current from Eq. (4.3) is 45 ± 23 nA in close agreement with experiment.

Using \( E = V/d_g \) (\( V \) the potential across the gap) the right hand side of Eq. (4.3) is viewed as a light power (I) dependent Ohmic conductivity so that we can define the gap resistance as:
and use this to calculate a resistance capacitance (RC) time constant for pixels with capacitance C. Since we are interested in the readout time for an entire line of pixels, we use a value of C that corresponds to the line length, which we take to be 20 cm. According to results in chapter 2 the pixel capacitance is 350 pF m\(^{-1}\) and hence the readout capacitance is 70 pF. We take the pixel rail gap (\(d_p\)) to be 5 \(\mu\)m, \(\eta = 0.2\) and \(y_p = 0.13\) \(\mu\)m. Finally we assume that the light power \(I\) available is 10 mW, a typical output of commercially available blue He-Cd lasers. The light intensity at the surface in this arrangement is about 10 times more intense than the maximum value used in the experiments of chapter 3. Using this brightness of light one finds the resistive line readout time to be \(\sim 2\ \mu\)s, sufficiently short for readout.

4.3.2 Operating PAS with intense readout light

In the previous section, the resistive line readout time was found to be short using a 10 mW laser. Increasing the laser power speeds readout but one might encounter limitations related to bimolecular recombination of carriers. As discussed in chapter 3, bimolecular recombination with carrier densities generated at the light levels used experimentally were not significant due to the spatial separation of the electrons and holes. However at higher intensity levels (about 10x those used in chapter 3) bimolecular recombination could start to dominate trapping effects and cause a saturation of current. Experiments need to be carried out to determine when bimolecular recombination starts to occur.

4.3.3 Possible extra noise sources
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In the PAS noise analysis of chapter 2 it was assumed that amplifier, kTC, and charge shot noise were the largest readout noise sources. It is known in the operation of FETs that 1/f noise (where f is temporal frequency) becomes dominant at low frequencies. It is believed that this type of noise has its origins in "surface" effects of the operation of the FET which one might suppose to be related to trapping effects. And with the slow optical charge switching time of several 100 ms in a PAS device (with surface trapping) the occurrence of a new type of 1/f noise must be considered a possibility. This has yet to be investigated, but even if it were to occur, could be circumnavigated by an AC signal processing chain that did not pass low frequency signals.

4.4 Pixel dark current leakage effects

The dark current leakage as presented and discussed in chapter 3 was measured between rails of 1 cm length. Therefore we can estimate the dark current leakage for a single 100 x 100 μm pixel which we shall take to have a length or perimeter of 400 μm. The dark current \( J_d \), was found to obey a fourth power law relation as a function of the average gap field \( E_{aq} \), i.e. \( J_d = b(E_{aq})^4 \), where \( b \) is an experimentally determined constant. If we take \( E_{aq} = V/d_g \) and utilize the relationship \( V = Q/C \), we can restate this relationship as:

\[
\frac{dQ}{dt} = -b\left(\frac{Q}{C d_g}\right)^4
\]  

(4.5)

where \( Q \), \( C \), \( V \), \( d_g \) are the pixel charge, pixel capacitance, pixel voltage and gap distance to the readout rail respectively. The value of \( C \) is 0.035 pF, the value of \( b \) is \( 1.20 \times 10^{-35} \) A (V/m)^4 and we take \( d_g = 5 \) μm. We can integrate Eq. (4.5) with limits of integration from 0 to \( t \) and we find:
\[ Q(t) = [Q(0)^{-3} + \frac{3bt}{(Cd)^4}]^{-1/3}. \quad (4.6) \]

where \( Q(0) \) is the charge at \( t = 0 \). Eq. (4.6) is plotted in Fig. 4.2 with a value of \( Q(0) = 5 \) pC which is equivalent to an exposure of \( \sim 50 \) mR. In comparison from chapter 2 the characteristic curve of PAS was calculated and plotted in Fig. 2.13 and the upper x-ray exposure limit of the dynamic range was set at \( \sim 150 \) mR (\( \approx 12 \) pC) arising from a restriction based upon an a-Se breakdown field assumed to be \( \sim 100 \) V \( \mu \)m\(^{-1}\). Inspecting the plot of Fig. 4.2 we see that a more realistic upper limit of the x-ray exposure is \( \sim 10 \) mR based upon the dark current leakage. The possibility of reducing leakage currents and reinstating the original estimate is discussed in section 4.8.

### 4.5 Reduction of surface trapping by materials engineering

We have determined that there are a large number of trapping states at the interface of a-Se and glass in our samples when the a-Se is evaporated on the glass substrate maintained at a temperature of approximately 50° C. The effects of surface states have been dramatically curtailed in c-Si devices by the use of SiO\(_2\). SiO\(_2\) is transparent (a necessary requirement for any anti-trapping layer in a light readout method) and when a c-Si/SiO\(_2\) interface is prepared properly the number of surface states present are reduced and surface recombination velocities \( S_r \) as low as 80 cm/s have resulted\(^5\). More recently certain etching techniques\(^3\) have reduced the \( S_r \) for c-Si wafers to as low as 0.25 cm/s. Therefore by analogy it would desirable to find a substance that is transparent and would generate few surface states when a-Se is deposited on it.

In passing we mention that the surface charge retention of freshly prepared a-Se surface increases in time after exposure to the atmosphere. This is probably due to the formation of trapping surface states due to chemical changes with oxygen. It is also known that the substrate
Fig. 4.2: Plot of signal pixel charge as a function of time after an instantaneous x-ray pulse of 50 mR. The leakage current rapidly reduces the charge to about 1/2 pC from an initial value of 5 pC.
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Temperature at the time of a-Se deposition affects the ability of a-Se to store charge. This again is probably related to the type of traps formed at the substrate/a-Se interface. The fact that the amount of trapping on the surface of a-Se has already been shown to be variable gives some reason to believe that an a-Se interface with fewer surface trapping states might be possible to engineer.

4.6 Moving charges under the surface

In Fig. 2.5(d) it is seen that a vertical field exists underneath the pixel and readout rails at their edges; the situation is presented conceptually in Fig. 4.3(a). Whereas the movement of charge directly at the interface plane (indicated by the horizontal field line) causes charges to be trapped in surface states and makes the development of a current difficult, it would seem the movement of charges underneath the surface would be a better choice. Referring to Fig. 4.3(a) the possibility arises of shining light at the edge of an electrode (transparent), generating carriers (holes in this case), which would then follow the field lines curving under the surface and towards the negative electrode.

The vertical field strength in a horizontal plane 0.5 μm below two horizontal planar rail and pixel electrodes (of infinite extent in and out of the plane of the paper) is shown in Fig. 4.3(b). The rail and pixel electrodes are 10 and 100 μm wide respectively and the gap separating them is 5 μm. The rail and pixel electrodes are at 0 and 50 Volts respectively and the fields were solved using the charge simulation methods of chapter 2. Inspection shows that indeed a strong vertical field exists for several μm away from the electrode edges.

In chapter 3 it was found that due to thermal diffusion of carriers, a field of strength \( kT/(y_p q) \) (where \( y_p \) is the penetration depth of the light into the photoconductor) must be present to move carriers away from a surface to avoid trapping. For a-Se this field strength is \( \sim 0.5 \text{ V } \mu\text{m}^{-1} \).
Fig. 4.3(a): Since charge transfer directly across the surface is hampered by a high density of surface traps one idea is to inject charges into the a-Se under a transparent electrode and have the charges follow the curved trajectory of the electric field lines to the other electrode.
Fig. 4.3(b): The vertical electric field 0.5 μm beneath a rail and pixel 10 and 100 μm wide respectively. The gap is 5 μm and the potential difference across the gap is 50 V.
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For relatively large x-ray exposures (> 10 mR) the vertical field would be sufficient to overcome thermal diffusion effects. However for smaller exposures the vertical field would not be sufficient. Additionally if a large amount of space-charge were to be vertically injected the charge would distort the vertical field profile and charges would tend to move towards the surface region.

4.7 Alternative PAS geometries that would avoid surface trapping states

The presence of surface states compromises the operation of PAS as originally conceived in chapter 2 where the free ballistic movement of charges was assumed. Therefore it would be natural to seek alternative PAS geometries that would move charges not at a surface but rather a short distance through a bulk or volume layer.

4.7.1 Pixellated dual photoconductor readout (PIXDP)

The first such possibility is shown in Fig. 4.4 and is called pixellated dual photoconductor readout, or PIXDP. The key features of the device are that it is a dual layer photoconductive arrangement with pixels twice the width of the readout rails. The conductive pixels are situated at the interface of the two photoconductive layers. The thick a-Se layer is for the absorption of x-rays and the charges generated in the thick a-Se layer are collected on a pixel electrode, as in the PAS approach. Directly above the pixel electrode is a thin switching photoconductive layer which could be a-Se or another photoconductor such as CdSe. At the top of the thin readout photoconductor are two conductive readout strips, one of which is transparent and the other opaque; one is connected to a charge amplifier, the other to ground. The image charge collected on the pixel electrode is shared primarily (capacitance to the bottom a-Se electrode is small) and equally with the two equal width readout rails. A short pulse of light, shorter than the transit time of charges across the photoconductive layer, causes discharge of half the charge on the pixel electrode, as
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Fig. 4.4: The PIXDP readout geometry moves charges a short vertical distance from a readout rail to a pixel electrode. The device has two photoconductive layers, a thin one for readout and a thick one for x-ray absorption and signal generation. The cross section region shown within the dashed lines constitutes a pixel.
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in the PID and PAS methods. Whereas the pixel charge (Q) is shared with the opaque readout rail a charge signal of strength 1/4 Q is developed on both readout rails, again analogous to the PID and PAS methods.

In the PIXDP approach, photogenerated charges at the interface of the transparent readout rail and the photoconductor move perpendicularly away from the interface towards the pixel electrode, hence minimizing surface trapping effects. However as pointed out in chapter 3 a minimum vertical field of strength $kT/(y_p q)$, where $y_p$ is the penetration depth of the light, is required to pull the charges away from the surface before they diffuse to the interface and get trapped. If the photoconductive layer were a-Se this would necessitate a vertical bias field of $\sim 0.5 \text{ V} \mu\text{m}^{-1}$ and would generate a bias noise. We now calculate this noise value and at what x-ray exposure level it becomes important.

In the PIXDP geometry the thickness of the photoconductive layer is small compared to the width of the pixel and readout electrodes. Therefore the capacitance is given accurately by the parallel plate formula. The field in a parallel plate capacitor is given by $V/d_g$ where $V$ is the potential and $d_g$ the plate separation. Furthermore $V = Q/C$ where $C = (A\varepsilon_\text{se})/d_g$ for a pixel of area $A$, and $E = V/d_g$. From this it follows that $E = Q/(A\varepsilon_\text{se}) = 1.79 \times 10^{18} \text{ Q [V m}^{-1}]$ and note that $E$ is independent of $d_g$. For a bias field $E_b$, to attain the value of 0.5 V $\mu$m$^{-1}$ we find a bias charge $Q_b$, of $\sim 0.3$ pC is required, which is equivalent to $\sim 2 \times 10^8$ charges. As in chapter 2 we assume the bias noise $N_{q_b}$ is related to the Poisson noise of the laser and therefore is given by $\sqrt{Q/q} \approx 1400$ q. Above what x-ray exposure levels does x-ray quantum noise exceed 1400 q? For a 1 $\mu$R exposure about 2 x-ray photons $\phi_x$ are incident on a 100 x 100 $\mu$m pixel. If we assume the mean x-ray energy is 35 keV, that $W_\text{ef}$ is 50 eV, then the gain $g$, is found to be $\sim 700$ q. We equate the x-ray quantum noise $N_{q_x}$ which is $\sqrt{\phi_x}g$ to $N_{q_b}$ and find that for $\phi_x > 4$ photons, or at exposure levels above 2 $\mu$R, the system is x-ray quantum noise limited.
The minimum readout time of a pixel is given approximately by \(d_g/(\mu E_0)\) where \(d_g\) is the thickness of the readout photoconductive layer. If the readout photoconductive layer were a-Se, \(d_g = 10\ \mu\text{m}\) thick, and additionally the polarity conventions were chosen to favour the involvement of holes in charge transfer, the minimum pixel read time would be \(-1\ \mu\text{s}\).

4.7.2 Non-pixelated dual photoconductor readout (NPIXDP)

For the PIXDP device it is necessary to etch and align two planes of electrode structures. The purpose of the pixel electrode structures is to maintain an equipotential over the pixel (defined to exist at the interface of the two photoconductive layers) so that charge can be shared equally between two readout rails situated very close to the pixel. This is essential for a signal to develop.

However the necessity for the pixel electrodes can be removed if the charge is simply stored at a thin trapping interface (eg. As\(_2\)Se\(_3\)) between the two photoconductors as shown in Fig. 4.5. The distance \(d_g\) is judiciously chosen so that the charge of an imaginary pixel, centred underneath the centre point (the point between the two readout electrodes), is shared approximately equally with the two rails. The required value of \(d_g\) will scale with the width of the readout rails, i.e. the wider the readout rails are, the larger \(d_g\) will need to be. The pixel pitch in both the NPIXDP and PIXDP approaches is set by the width of two readout rails.

4.8 Future experiments and theoretical work

In order to make the PAS readout method operate as delineated in chapter 2, two primary things need to be changed: (1) the number of surface states in the readout gap must be substantially reduced and (2) the leakage current from pixel electrodes requires reduction.

The first problem is most certainly only one which can be solved by empirical methods, guided by some of the ideas presented in the previous sections. Therefore the ability to evaporate
Fig. 4.5: The NPIXDP readout geometry also has two photoconductive layers but in this arrangement there are no pixel electrodes and signal charge is trapped by a thin layer of arsenic triselenide at the interface between the two photoconductors. The use of a thin trapping layer obviates the need for a second layer of electrodes but the choice of $d_g$ must be carefully considered.
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a-Se on varying substrates (at different temperatures) in a quick and timely fashion is needed in order to quickly test the surface photoconductivity of freshly prepared samples. Refined experimental techniques based on the methods of chapter 3 should be able to rapidly quantify the nature of the trapping states from an analysis of the surface photoconductivity.

The second problem will also require empirical testing of different electrode materials in order to find potential candidates for "blocking electrodes" (those which do not inject charges into the photoconductor and hence sharply limit leakage). Conventional wisdom attributes the success of certain materials as blocking as arising from the effects of their different work functions compared to the photoconductor.

However it is likely that most of the leakage in a PAS electrode geometry is generated at the edges of the electrodes where the fields are very high. It is likely that the choice of a proper blocking material will be a necessary step to reduce leakage current but not the only or sufficient step required. A method of reducing the high electric fields at the electrode edges is probably required. This might be achieved through electrode design or the introduction of a "doping" material that would reduce the electric field near the electrode edges.

It would also be of theoretical interest to determine if the fourth power law dependence of dark current can be explained by space-charge effects occurring at the edges of the electrodes.

Fortunately it has been found that a resistive mode of operation of PAS appears feasible based upon predictions of Eq. 4.4. Experimental positive or negative confirmation of the expected effects of bimolecular recombination (reducing the expected current) at the higher light levels used for resistive readout would be useful.

4.9 Final summary of thesis

Chapter 1 outlined the requirements of a digital radiographic system. The potential advantages
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of a well implemented digital radiography system over current screen-film methods were outlined. Approaches currently being researched to achieve digital radiography were introduced and one of these, the PID method previously investigated experimentally and theoretically by the author, was shown to have limitations at low exposure levels due to a long readout time and bias noise problems.

In chapter 2 the theoretical characteristics of a structurally simple digital radiographic system method (PAS), based upon photoswitching charges at the interface of a-Se and an insulator to narrow readout rails, were determined. The analysis assumed that the photoconductive properties of a-Se were those of the "bulk". The design goal of PAS was to overcome the readout time and bias noise problems of PID approaches and it was found that the PAS method in principle solved these problems.

In chapter 3 experimental results of photoconductivity at an a-Se glass interface were presented. It was found that the photoconductivity was far weaker and of a different qualitative nature than expected from calculations of chapter 2. Bulk photoconductivity of the samples was also carried out and showed that the a-Se had nominal properties. Dark current measurements were also performed and showed an increase as the fourth power of the average electric field in the gap separating the electrodes.

A new theory was constructed in chapter 3 to explain surface photoconductivity in a-Se. The theory explains in detail the surface photoconductivity of a-Se as arising from the presence of a high density of deep surface trapping states for both electrons and holes. The theory explains adequately all basic experimental observations both qualitatively and quantitatively. The theory also explains the reduction, at low electric fields, of the photogeneration efficiency observed by Pai and Enck.

In chapter 4 the effects of surface trapping upon readout time were calculated for the
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Arrangement leading to the highest photoconductivity: full illumination of the readout gap. It was found the photoconductivity behaves as an illumination dependent resistance. From the value of this resistance, for a 10 mW laser, and the calculated capacitance of a line of pixels from chapter 2, it was found the resistive readout time could be as short as several µs. On the other hand the discharge effects of dark current on signal were calculated and found to be very fast, causing substantial reduction of the signal in about 50 µs for signal charges arising from a 10 mR or greater exposure. In conclusion it is clear that both surface and leakage effects should be reduced in order to allow the operation of PAS as conceived in chapter 2. However, assuming that leakage effects can be addressed and that bimolecular recombination does not become significant at light intensities greater than those investigated in chapter 3, it appears that a resistive mode of operation using full gap illumination is promising.

References


