Wide bandgap semiconductors for harsh environment imaging: temperature dependence of p-n junction detector efficiency

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Wide Bandgap Semiconductors for Harsh Environment Imaging:
Temperature Dependence of P-N Junction Detector Efficiency

By

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Bachelors of Science, Physics, RIT

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in the Chester F. Carlson Center for Imaging Science Rochester Institute of Technology

June 4, 2007

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Temperature Dependence of P-N Junction Detector Efficiency

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*Temperature Dependence of P-N Junction Detector Efficiency*

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Danielle Merritt

Submitted to the
Chester F. Carlson Center for Imaging Science
in partial fulfillment of the requirements
for the Master of Science Degree
at the Rochester Institute of Technology

Abstract

The majority of image detectors to date have used silicon photodiode arrays for light capture and image formation. However, as imaging is performed in increasingly harsh environments, conventional silicon arrays begin to reach their physical device limitations and fail. Harsh imaging conditions include short wavelengths, high temperatures, and/or high radiation conditions. To aid future detector development, the theoretical energy-conversion efficiency of wide-bandgap semiconductor materials, which are long known for their favorable properties in harsh environments, has been studied. It has been hypothesized, but not shown until now, that wide bandgap semiconductors have better energy-conversion efficiencies at higher temperatures than conventional semiconductor materials. The basic element of the photodiode, the p-n junction, is investigated using fundamental physical equations including the short-circuit current, open-circuit voltage, and energy-conversion efficiency, as a function of temperature and material. The results of several wide-bandgap materials (i.e. GaP, SiC, and GaN) are compared to silicon. The limitations of current silicon detector technologies (CCDs) and the potential of these wide-bandgap semiconductors as imaging and non-imaging devices (e.g. solar cells and alpha-voltaic batteries) are presented. Experimental results showing the normalized to Si energy-conversion efficiency as a function of temperature for Si, InGaP, and SiC substantiate the theoretical conclusions that wide bandgap semiconductors offer better efficiencies at higher temperatures than narrow bandgap semiconductors.
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Chapter 1

Introduction

Harsh environment imaging is exactly as it sounds, imaging with sensors in harsh environments. These environments include short wavelengths, high temperatures and high radiation backgrounds. Conventional detectors, such as silicon charge coupled devices, have inherent material properties that cause the detectors to fail in these hostile environments. A great deal of research is being done to improve detector technology to perform more efficiently in harsh environments, including modifying conventional detector designs as well as the use of new detector materials.
Chapter 1. Introduction

1.1 Harsh Environments

1.1.1 Short Wavelengths

Figure 1 illustrates the electromagnetic spectrum, highlighting the subdivisions of interest for harsh environment imaging: X-ray and UV (ultra-violet) radiation. X-rays begin at 10nm and extend down to the smallest wavelengths. UV wavelengths range from 10nm-400nm. Extreme UV (EUV), ranging from 10nm-100nm, corresponds to the highest energy UV photons. Materials used for EUV applications must exhibit a high resistance to radiation damage and be free of defects. Far UV (FUV), also referred to as Vacuum UV (VUV), ranges from 100nm-200nm. Air is opaque at these wavelengths, therefore experiments and operations conducted in this range need to be preformed in vacuum or inert gas to avoid absorption by air. Deep UV (DUV) ranges from 180nm-280nm and is the deepest part of the UV spectrum where work can be done in atmospheric conditions without radiation side effects. Mid-UV (MUV) ranges from 280nm-315 and Near-UV (NUV) ranges from 315nm-400nm (Li, Flora, 2005).
1.1.2 High Temperature and Radiation

Most conventional silicon devices are not able to operate at temperatures above 250°C, especially when these high operating temperatures are combined with other harsh environments such as high-radiation. High-temperature circuit operation from 350°C to 500°C is desired for use in aerospace applications (turbine engines), nuclear power instrumentation, satellites, space exploration, and geothermal wells (Pearton2, 2000). For example, a detector imaging close to the sun at the surfaces of Mercury or Venus, will have to operate at temperatures exceeding 700K and 750K, respectively (Hey, 2002). Imaging at these locations will result in increased cosmic ray events, increasing the potential for radiation damage.

1.2 Harsh Environment Detector Characteristics

One class of image detectors is photoelectric image detectors. Photoelectric detectors convert incident photons into an electrical signal. The useful wavelength range and spectral sensitivity of such a detector vary widely with the choice of detector material (Grossweiner, 1994). Two typical
subclasses of photoelectric detectors are Solid State and Photoemissive detectors. Solid-state devices, which absorb photons using a semiconductor, typically have sensitivities over a broader range of wavelengths than photoemissive detectors that use photocathodes which have sensitivities tailored to specific wavelength intervals. Figure 2 illustrates some of the inherent properties of each (Joseph, 1999).

![Image Sensors](image)

**Photoelectric**
- Photoemissive
  - UV sensitive
  - No cooling
  Examples: MCP, EBCCD
- Silicon based
  - Visible -IR sensitive
  - Dark Current, cooling
  Example: CCD
- Wide Bandgap
  - Solar blind UV sensitive
  - No cooling
  Examples: GaN, SiC

**Photographic**
- Solid State

Figure 2. Schematic of two subclasses of photoelectric detectors: solid state and photoemissive (adapted from Joseph, 1999).

Considering the Solid-State device, there are several fundamental detector properties required for harsh environment imaging:

- High Detective Quantum Efficiency (DQE),
- High Local Dynamic Range (LDR),
- Low background noise/dark current/read noise,
Chapter 1. Introduction

- Radiation hardness and resistance to Si-typical radiation deterioration effects,
- Ability to operate at high temperatures with low dark current,
- Low/no sensitivity to light of visible wavelengths, in other words "solar blind".

Other parameters including weight, volume, and required power capabilities can also be very important for specific applications.

Quantum efficiency (QE) is defined as the number of electrons generated in the device per incident photon. Ideally, QE would be 100%; or one electron-hole pair generated per incident photon. QE does not take into account many parameters that could negatively affect the outcome of generating electron-hole pair within a device, such as surface reflection. **Detective Quantum Efficiency (DQE)**, or internal efficiency, takes these losses into account. Most visible wavelength detectors have reflection efficiencies less than 5% so QE and DQE are approximately equal. However, visible wavelength devices used for short wavelength (UV and X-ray) imaging are plagued by reflection losses, resulting in a substantial difference between QE and DQE. For example, Si is reflective in the UV and short end of the visible wavelengths, with values as high as 70%, making it a poor choice for UV detection, as shown in Figure 3. It is important to take DQE into account when considering detector material and operating conditions.
Astronomical objects of interest often emit $10^4$-$10^8$ visible photons for every FUV photon. If the detector used is not solar blind, the resulting image will contain an enormous visible background that will substantially decrease the signal to noise ratio (SNR) of the UV signal. Even if a filter is used to block the unwanted visible wavelengths, a significant amount of visible wavelength leakage may still occur. In either case, with or without the solar blind filter, the DQE is reduced.

Local dynamic range (LDR) is defined as the maximum level of flux that can be accommodated in a small area of the detector minus the smallest level that is still three standard deviations above the background noise and read noise. LDR is different than Global Dynamic Range (GDR), the total flux rate spread over the whole detector. LDR becomes important since most UV astronomical scenes have most of the light in relatively few pixels and are generally faint (Joseph, 1999).
Dark current noise is the current that is present in the absence of light or signal, as a result of the detector's thermal energy. This noise current is captured by the detector and counted as signal, decreasing signal to noise ratio (SNR). As exposure time increases and/or imaging environment temperature increases, dark noise increases. Detectors can be cooled to reduce this effect. There is a tendency for contaminants to condense on cooled detector surfaces, even in the vacuum of space, which reduces the sensitivity further (Ulmer, 1995). Ideally, the dark current noise should be reduced to a point where its contribution is negligible over a typical exposure time. In some cases, sensors have enough dark noise to warrant dark frame calibration. For this calibration a "dark" image is taken, with no light exposure that allows the dark signal to be quantified over some exposure time. To account for statistical variations, multiple dark images are taken and averaged. The average dark signal can later be subtracted from real images to eliminate dark noise contributions (Li, 2005).

1.3 Conventional Harsh Environment Image Detectors

1.3.1 Silicon Charge Coupled Devices

Currently, the most common solid-state detectors are Si-based CCDs. It is known that CCDs have excellent sensitivity in the visible and near-infrared (NIR) portion of the electromagnetic spectrum (Joseph, 1999).

Front-illuminated CCDs tend to have good red QE but poor short wavelength QE. This is partly because the poly-silicon gates absorb blue and shorter wavelengths. The gates can be thinned to reduce absorption, but other methods exist to help with this problem. CCDs can be coated with
lumigen which absorbs blue and shorter wavelengths and then fluoresces yellow which CCDs are very sensitive too. There are some drawbacks to this technique, mainly that the fluorescence occurs in all directions creating unwanted cross-talk between pixels. Transparent gates can be used such as ITO (Indium Tin Oxide); however, these heavy metals can diffuse into the silicon and act as electron traps and recombination centers.

A more promising solution is back-illuminated CCDs. By illuminating from the back, all of the gate-related problems are eliminated. The bulk silicon is etched away to the epi-layer of silicon thinned to about 10-15 microns for proper absorption. The backside is then coated with metal, silver or platinum, and negatively charged to reduce any traps created by a roughly etched backside (Ulmer, 1995). Figure 4 illustrates a front and back-illuminated CCD and the QEs of each (Inoue, 1997).
1.3.2 Micro-channel Plate Detector

To overcome some of the limitations of CCDs, especially at short wavelengths, Micro-channel plates (MCPs) are introduced that precede the CCD in the optical path (Howell, 2000). MCPs amplify the incident light using two-dimensional periodic array of very-small diameter glass capillaries (channels) fused together and sliced in a thin plate. A single incident photon enters a channel and emits an electron from the channel wall. The electron is accelerated by an electric field and continues to strike the channel surface, producing additional electrons per strike until the end of the channel. Each additional electron continues in this manner; when it hits the wall it produces more electrons. MCPs can produce up to approximately 500,000 electrons per incident high energy photon and this electric cloud strikes a phosphor coated photocathode producing
Chapter 1. Introduction

visible photons that are collected and imaged by a CCD. MCPs operate at high voltages and are inherently solar blind as they require high energy photons for activation (Howell, 2000).

Figure 5. Micro-channel plate intensifier (Waynant, 2000).

Figure 6 illustrates the solar-blind efficiencies of CCDs and MCPs. Unfortunately, when a filter is introduced to make a visible CCD solar blind, the QE drops below 10% in the range of 0-200nm. MCPs have better QE for short wavelength detection. The AlGaN (aluminum-gallium-nitride), a wide bandgap semiconductor, solid-state detector, also has potential as a short wavelength detector as seen plotted with the dotted line.
Chapter 1. Introduction

Solar-Blind Efficiencies

Figure 6. Solar-blind UV DQEs of various detectors (Ulmer, 1995).

1.4 Limitations of Conventional Image Detectors

Both CCDs and MCPs exhibit shortcomings that severely limit their performance. The major points are summarized here:

- CCDs are most sensitive in the visible and IR and less sensitive for UV wavelengths. When filters are introduced to make them "solar blind", most of the unwanted visible wavelengths are attenuated, but some of the desired UV radiation is also attenuated.

- CCDs have high dark current, even at room temperature. To reduce the dark signal, CCDs must be operated at low temperatures and therefore cooling systems must be added. This is technically challenging and costly. The cold detector surface can create a cold trap for condensable contaminants inside the instrument, leading to very unstable performance due to contaminant build-up on the sensitive surface (Joseph, 1999).
Chapter 1. Introduction

- Bake-out resources are needed to frequently drive off the volatile condensable material from cooled detector surfaces which can lead to additional mass, higher cost, and/or more power consumption. Furthermore, organic contaminants (including hydrocarbons) have longer residence times on the cold surface. They may polymerize under UV radiation and cause irreversible degradation of the detector operations (Schühle, 2004).

- CCDs are generally not "radiation hard". The ionizing radiation of the space environment leads to "cosmic-ray hits" (points and streaks) obscuring the images. In addition, non-uniform radiation damage can cause a non-uniform spatial response of the array, further obscuring the image.

Microchannel plates have additional drawbacks listed below.

- MCPs need high voltage for amplification.
- MCPs have limited resolution due to the pore size of the channels, to about 10µm.
- MCPs have limited dynamic range due to gain saturation at high counts rates.
- MCPs lead to distortion of the image due to the imperfect image transfer between the photocathode and the anode by the residual alignment errors between the channels and the gap between the MCP and the anode (or the CCD) (Joseph, 1999).
- The response of MCPs is unstable due to scrubbing (i.e. their gain reduces continuously during usage). This makes the calibration difficult to maintain. The high voltage must be increased to compensate for scrubbing (Schühle, 2004).
1.5 Possible Solutions to Limitations of Current Harsh Environment Detectors

1.5.1 Cooling and Mechanical Shielding

As it was mentioned previously, cooling can be implemented to reduce the dark current detectors. With effective detector cooling, the effect of dark current can be negligible. As a simple rule of thumb, detector noise can be cut in half for every 20K decrease in temperature. The extent of cooling depends mostly on the image exposure time desired and the maximum acceptable signal to noise ratio. CCDs most commonly use liquid nitrogen Dewar systems or attached Peltier coolers to cool the system, both of which increase size, weight, and cost of the system (Bard, 2004).

Like cooling systems, mechanical shielding offers detectors physical protection and increased device efficiency. Mechanical shielding protects against harmful radiation. Pfeffermann et al presented results showing that CCD detectors can be shielded quite efficiently with low Z materials from fluorescent X-rays generated by cosmic rays in the material surrounding the detector (Pfeffermann, 2004). This prevents damage to the detector in space missions with cosmic ray hits events.

As Pfeffermann showed shielding CCDs is possible, but it also introduces added weight, increased design time and cost. These solutions still do not completely protect the detector from the long-term effects of high radiation and temperature.
1.5.2 Nanotechnology

Another potential solution to harsh environment imaging is the introduction of quantum dots (QD) to detectors. An NREL (National Renewable Energy Laboratory) team, led by Arthur Nozik, found that quantum dots produce as many as three electrons from one high energy photon of sunlight.

In 2000, Nozik predicted the multiple exciton generation (MEG) process of QDs. In 2004, Richard Schaller and Victor Klimov of Los Alamos National Laboratory in New Mexico were the first to demonstrate the electron multiplication phenomenon predicted by Nozik, using quantum dots made from lead selenide. For example, solar cells based on quantum dots theoretically could convert more than 65 percent of the sun's energy into electricity, approximately doubling the efficiency of solar cells (Ellingson, 2005).

While the QD focus here is on photovoltaic solar cells, a clear comparison with detector technology is obvious. Using the MEG, QD detectors would have better quantum efficiency at lower intensities which is important for faint UV observations.

The main advantages of quantum dots are: (1) lower dark current due to the 3D-confinement of carriers, (2) possibilities for higher operating temperature, which consequently will lead to less expensive systems (no cooling system needed), (3) absorption of radiation at all angles of incidence since the electrons are confined in all directions, which will lead to simpler fabrication process, (4) longer lifetime of excited carriers than in a CCD, which will increase the probability for an excited electron to contribute to the photocurrent and will therefore increase responsivity, (5)
Chapter 1. Introduction

radiation hardness, and (6) design characteristics are favorable for reduced volume and weight (Acreo, 2005).

1.5.3 Wide Bandgap (WBG) Semiconductor Materials

Current Si-based CCDs generally have poor efficiency in harsh environments. They can not operate at temperatures above 300°C, are not solar blind, and are not inherently radiation hard. Cooling and mechanical shielding improves efficiency but have inherent drawbacks. Quantum dots provide only a theoretical solution to harsh environment image detectors. However, wide bandgap semiconductors offer a valid solution as harsh environment image detectors by overcoming many of the Si-CCD limitations and disadvantages previously listed. Wide bandgap semiconductors are more sensitive to X-ray and UV spectrums, can withstand high operating temperatures, and are generally more radiation hard than Si, along with other favorable harsh environment properties. They will be more cost effective than previous detectors by sparing the development and weight of high voltage power supply, cooling hardware, radiation shields and bake-out resources (Hochedez, 2003).

In addition to the imaging, other industries such as aerospace, automotive, petroleum are continuously pushing the development of wide bandgap devices that are tolerant of increasingly hostile environments. Since silicon carbide (SiC) technological development is the most mature of the wide bandgap semiconductors, it appears that most high-temperature, high-power electronic devices will be fabricated from that material. Gallium nitride (GaN), another wide bandgap semiconductor, is still technologically immature but also has inherently favorable properties, making a promising semiconductor materials for harsh environment applications (Razeghi, 1996).
Chapter 2

Theory

2.1 Wide Bandgap Semiconductors

Some of the advantages of wide bandgap semiconductor as imaging detectors are listed below:

- Wide bandgap detectors operate at higher temperatures,
- Cooling systems are not needed and as a result contamination is reduced thereby eliminating heating resources for contamination bake-out further reducing cost/weight/power consumption,
- Detectors are inherently solar blind making them promising candidates for UV and X-ray detection,
- Compact crystal networks provide better radiation hardness: the smaller atomic numbers offer a smaller cross-section to damaging radiation,
Chapter 2. Theory

- Greater resistance to electrical breakdown: the field strength can be higher, and the pixels can be in the sub-micrometer range, increasing image resolution, an order of magnitude smaller than silicon-based detectors,
- Higher carrier velocities (Hochedez, 2003),
- High thermal conductivity implying lower thermal resistance which means that the device can transfer unwanted heat out more easily, resulting in a slower device temperature increase.

2.2 Wide Bandgap Semiconductor Supporting Research

While the high temperature applications of SiC had been known for years, the recent availability of silicon carbide had made possible the realization of a large variety of devices intended for specific applications including related device elements such as: ohmic contacts, insulating layers, interconnections, encapsulation techniques, etc. Chelnokov and Syrkin reviewed two main problems which played key roles in the development of SiC based high temperature electronics: (1) physical problems of the real high temperature properties of SiC, and (2) physical and technical problems of the high temperature related electrical parts.

In common semiconductor electronics, the working temperature, $T_w$, of p-n junctions is the temperature where the reverse current at a fixed reverse voltage, close to the breakdown voltage, does not exceed the chosen initial current. In other words, the maximum temperature before thermal electrons dominate the current of the device. This was used to calculate theoretical parameters of SiC. $T_w$ increases linearly with semiconductor bandgap, as shown in Figure 7. This figure illustrates the potential of wide bandgap semiconductors as high temperature devices.
Chapter 2. Theory

Another thermal characterization emphasized was the temperature of thermal stability of the material. The maximum value of this temperature is the melting temperature, \( T_m \), and minimum value is the Debye temperature, \( T_D \). A high Debye temperature signifies strong bonds, high melting temperatures, low thermal expansion, high strength and elastic moduli (Waynant, 2000).

Figure 8 shows the relationship of \( T_w \) and \( T_D \) for semiconductors. The semiconductors of interest were separated into four groups: (1) Ge, Si, BP, 3C-SiC with \( T_D = 1.5 \ T_w \), (2) 6H-SiC, 4H-SiC, C (diamond) with \( T_D = T_w \), (3) GaAs, GaP, GaN, AlN, BN with \( T_w = 1.5 \ T_D \) and (4) GaAs\(_{1-x}\)P\(_x\), CdS, ZnS with \( T_w = (2.5-4) \ T_D \). Group four has low thermal conductivity and is not successful for semiconductor devices. Group two has high thermal conductivity, greater than group one or group three, therefore good for high temperature applications (Chelnokov, 1997).

![Figure 7. Operating temperature vs. Bandgap (Chelnokov, 1997).](image)
Chapter 2. Theory

Vest et al explored the use of wide bandgap semiconductor materials in vacuum ultraviolet (VUV) radiation. For this research, National Institute of Standards and Technology (NIST) collaborated with several developers of new detector technologies, particularly in the characterization of wide bandgap semiconductors that can be used as solar-blind, solid state photodiodes; mainly space-based research and related technology development.

The broadband visible response of Si photodiodes is a major problem in using these detectors for VUV signals in solar physics applications or other environments with high visible radiation backgrounds. Vest, et. al., measured the QE of GaN and SiC photodiodes in 5x5mm\(^2\) and 10x10mm\(^2\) configurations and the spatial uniformity of response of the 5x5mm\(^2\) GaN samples. The spatial uniformity of response for the 5x5mm\(^2\) GaN varies \(-4\%\) over the active area (Vest, 2005).
Figure 9 shows the QE Vest, et. al., measured, where both GaN and SiC have QE peaks at approximately 225nm, showing good results for VUV detection.

![Graph showing quantum efficiency of wide-bandgap photodiodes](image)

**Figure 9.** The quantum efficiency of 10mm² wide-bandgap photodiodes made from GaN and SiC (Vest, 2005).

Kung, et. al., also researched GaN, AlN and GaAIN for the primary active materials in UV solar blind photo-electronic detectors. For their experiments, high quality AlN and GaN was grown on sapphire. They measured the response in the back illumination mode where the responsivity peaked at 350nm.

They noted that the response could be improved by a number of methods: (1) making a thinner n-GaN layer or using a heterojunction; (2) improving the geometry; and, (3) fabrication of better contacts on the n- and p-type GaN layers. Kung, et. al., also made a device with an improved broadband response. Briefly, this device is an n-type GaN photo detector made by placing metal
contacts on the top surface of a GaN layer that has been deposited on a sapphire substrate. The responsivity of this device was measured via front illumination, having a flat peak from approximately 350-360nm with a quantum efficiency of 80% (Kung, 1996).

Blank, et. al., noticed that most of the research conducted on short-wave QE of 4H-SiC Schottky UV detectors had been carried out only at room temperature where only detector stability was of concern. The group investigated the detailed temperature dependence of the quantum efficiency of the photoelectric conversion process for UV detectors over a large temperature (78–400K) and wide photon energy (3–6 eV) range. The aim of the research was to determine: (1) the mechanism of the photoelectric conversion process and (2) the temperature stability of different UV detectors.

The main results of Blank, et. al., showed that Schottky photo detectors based on GaAs, GaP, 4H-SiC have increasing quantum efficiency with increasing temperature over the whole photon energy range; whereas p-n photo-detectors based on GaAs and Si have quantum efficiencies that are independent of temperature and independent in the region of intrinsic absorption. In the future, they plan to investigate the influence of temperature on the photoelectric conversion process in different ultraviolet photo detectors. They listed tasks including the determination and explanation of: (1) temperature dependence of the quantum efficiency for p-n and Schottky photo-detectors based on GaN; and (2) temperature dependence of the quantum efficiency of shallow p-n photo-detectors (based on 4H-Si); and external electric field influence on the quantum efficiency for UV photo-detectors (Blank, 2003).

In 2004, Schühle, et. al., worked on a project called “Blind to Optical Light Detectors” (BOLD), and investigated devices made of AlGa-nitrides and diamond. They examined the responsivity
measurements extending from the visible down to extreme UV wavelengths for these devices. The initial responsivity measurements achieved visible-to-UV rejection rates that exceeded four orders of magnitude, but they anticipated still higher rates in the future due to thinning techniques and improvement of crystal quality. For energies above the bandgap, the responsivity shows a quite flat response (wavelength range 275-375nm).

The experiments were performed using three GaN Metal-Semiconductor-Metal (MSM) photodiodes with 2, 4, and 7μm wide electrodes and active areas of 500 × 500 μm². The GaN Schottky diode structures showed a very good response throughout the whole range from 40 nm to 250 nm; however the photo response diminished in the 130-250 nm range. As the absorption coefficient increases in the same range, the responsivity decreases. The origin of this reduction seems to be related to surface characteristics involving oxide formation or high surface recombination rates. Schühle, et. al., list two phenomena that must be taken into account as a response to this. First, there is a change in the absorption coefficient behavior since it begins to decrease with the photon energy. Second, the photon energy is higher than the ionization energy (the average amount of energy given up by the incident radiation in the process of generating a single electron-hole pair), which can cause the creation of multiple electron-hole pairs by an incident photon. Schühle, et. al., notes that these processes have to be carefully studied in order to optimize the spectral response in this photon energy regime.

Proving wide bandgap semiconductors' potential, Schühle, et. al., fabricated small arrays to go aboard the LYRA Instrument. The LYRA instrument (Lyman-alpha Radiometer) is a small, compact instrument that will monitor the solar irradiance at four spectral regions of the UV, taking advantage of the wide bandgap materials as their sensing devices. The goal of the LYRA is to
demonstrate the superiority of the GaN arrays with respect to VUV sensitivity, solar blindness, calibration stability, and radiation hardness. The LYRA will be used on the Proba-2 mission of ESA. Proba (Project for on-board autonomy) was conceived for the purpose of demonstrating new on-board technologies (Schühle, 2004).

Since 2000, radiation detectors have been manufactured and tested which demonstrate excellent results in neutron, alpha, gamma and X-ray detection. In 2004, Bertuccio, et. al., began research funded by INFN (Istituto Nazionale di Fisica Nucleare) and MIUR (Italian Ministry of University and Research) focusing on developing technology to manufacture SiC detectors for spectroscopy, X-ray imaging, and studying the properties of this new class of detectors. In particular, their aim was to demonstrate the feasibility of high-resolution X-ray spectroscopy at room and high temperatures using SiC and its high Schottky barriers.

One problem that Bertuccio, et. al., were trying to overcome with SiC verses present Si detectors is the need to cool the system in order to reduce noise due to leakage current. On the basis of fundamental noise analysis of spectroscopy systems, they evaluated the expected energy resolution for 4H–SiC detectors. Figure 10 shows the results of the simulations: the higher performance of SiC with respect to Si is significant above room temperature, especially for relatively large area detectors in which the leakage current constitutes the main noise source. SiC also has the lower slope of noise with respect to temperature variations.
Bertuccio, et. al., acknowledge that the limit of the presented detectors is related to their small depletion layer thickness due to a relatively high unintentional doping \((10^{14} \text{ cm}^{-3})\) and to the epitaxial layer thickness \((70 \ \mu \text{m})\). Recent SiC epitaxial growth technology has achieved doping levels around \(10^{13} \text{ cm}^{-3}\), opening new possibilities. Semi-insulating SiC wafers constitute an interesting alternative and will be examined in their future work (Bertuccio, 2004).

CERN (European Organization for Nuclear Research) requires a detector upgrade with detectors able to operate in harsh radiation environments at fluences of \(10^{16} \text{ fast hadrons/cm}^2\) for a project called RD50. These are needed for use in nuclear reactors and position sensitive detectors for...
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particle beams and advanced light sources. In particular, experiments at the CERN Large Hadron Collider (LHC) will be subject to fluences of greater than $10^{15}$ fast hadrons/cm$^2$.

As of October 2005, the Glasgow team had successfully made and tested SiC and GaN devices for the RD50. These were Schottky devices on commercially available materials from Okmetic and Cree. Other materials included bulk GaN from Vilnius University, Lithuania, as well as SI (semi-insulating) epitaxial GaN detectors made at Tokushima University, Japan. Standard fabrication methods were used to produce test structures and the resultant detectors were electrically characterized pre- and post-irradiation by performing IV (Current-Voltage) measurements and CCE measurements.

All of the detectors were irradiated with pions, protons, X-rays, and neutrons. The results of the research showed that vanadium doped SiC had low CCE because of charge recombination at vanadium centers. Initial measurements of SI-SiC showed that undoped SiC had close to 100% CCE. Irradiated vanadium doped SiC showed little degradation under pion influences. The doped SiC detectors also operated effectively at relatively low bias voltages resulting in lower power consumption as compared to Si detectors. Initial testing of SI-GaN detectors resulted in CCE values of 5% after fluences of $10^{16}$/cm$^2$ protons and neutrons. Initial thinking is that the CCE could be increased by cooling the detector (Grant, 2004).

The results of this study find that wide bandgap semiconductors show promise for effective and efficient operation in harsh environments including high temperatures and short wavelengths. Glasgow also proved that SiC is a very radiation hard material.
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2.3 Wide Bandgap Semiconductor Properties

The physical properties of these semiconductors will be explored along with other parameters used to characterize their value. Some of the more popular wide bandgap semiconductor materials and Si are listed in Table 1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Si</th>
<th>6H-SiC</th>
<th>4H-SiC</th>
<th>GaN</th>
<th>GaN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandgap Energy (eV)</td>
<td>1.12 (Luque, 2003)</td>
<td>3.0 (Goldberg, 2001)</td>
<td>3.23 (Goldberg, 2001)</td>
<td>3.2 (Bougrov, 2001)</td>
<td>3.39 (Chow, 1996)</td>
</tr>
<tr>
<td>Crystalline Structure</td>
<td>Diamond (Luque, 2003)</td>
<td>Wurtzite</td>
<td>Wurtzite</td>
<td>Zinc Blende</td>
<td>Wurtzite</td>
</tr>
<tr>
<td>Debye Temperature (K) (Byrappa, 2003)</td>
<td>645</td>
<td>1200</td>
<td>1200</td>
<td>710</td>
<td>710</td>
</tr>
<tr>
<td>Melting Point (°C)</td>
<td>1412 (Luque, 2003)</td>
<td>3103 (Tairov, 1988)</td>
<td>3103 (Tairov, 1988)</td>
<td>2500 (Porowski, 1997)</td>
<td>2500 (Porowski, 1997)</td>
</tr>
<tr>
<td>Electric Breakdown Field (10^6V/cm)</td>
<td>0.3</td>
<td>0.6 (Goldberg, 2001)</td>
<td>0.6 (Goldberg, 2001)</td>
<td>5 (Chow, 1996)</td>
<td>5 (Chow, 1996)</td>
</tr>
<tr>
<td>Thermal Conductivity (W/cmK)</td>
<td>1.3 (McGuire, 1988)</td>
<td>4.9 (Goldberg, 2001)</td>
<td>3.7 (Goldberg, 2001)</td>
<td>1.3 (Chow, 1996)</td>
<td>1.3 (Chow, 1996)</td>
</tr>
</tbody>
</table>

Table 1. Physical properties of popular wide bandgap semiconductors and silicon at 300K.
Chapter 2. Theory

First and foremost, the most obvious parameter to investigate when considering high temperature applications is the melting point of the material. Si melts at 1685K, almost 2500K less than SiC and 1000K less than GaN. Si would melt before being able to image in most harsh environments.

Semiconductors with wider bandgaps can operate at higher temperatures, and have higher breakdown fields, resulting in devices that can function at higher voltages. Looking at Table 1, it can be seen that the electric breakdown field for wide bandgap semiconductors is much larger than Si. For example, the breakdown voltage of a diode is (Tolbert, 2003):

\[ V_n = \frac{\varepsilon_r E_x^2}{2qN_d} \]  

Equation 1

Where q is the charge of an electron, \( N_d \) is the doping density, \( \varepsilon_r \) is the dielectric constant and \( E_x \) is the electric field.
Using Equation 1, the breakdown voltages of diodes made of the materials listed in Table 1 assuming the same doping densities and the results are shown in Figure 11 normalized to the breakdown voltage of a Si diode. As can be seen, 6H-SiC, 4H-SiC, and GaN offer a higher breakdown voltage; 56, 46, and 34 times as great as a Si diode. With a higher electric breakdown field, more doping can be applied to the materials, further widening the gap between the upper breakdown voltage limits of the wide bandgap semiconductors compared to silicon. Another result of the higher doping density is the reduction of the width of the drift region. The width of the drift region is expressed as:

\[ W \approx \frac{2V_B}{E_C} = \frac{\varepsilon_r E_C}{qN_d} \]

Equation 2
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Si has the maximum drift region as expected. As it is seen in Figure 12, overall width increases with increased voltage.

![Graph of drift region width vs voltage](image)

Figure 12. Width of the drift region for each material at different breakdown voltages.

Another parameter to highlight in Table 1 is the thermal conductivity. It indicates the devices’ ability to get rid of unwanted thermal energy. This is a useful property, indicating the high operation temperature capability of a device. SiC has the best thermal conductivity of the semiconductors listed in Table 1. Interestingly, GaN has poor thermal conductivity, comparable to Si.
Table 2. Normalized Figures of Merit for Semiconductors of interest (Tolbert, 2003).

Table 2 gives a brief glimpse of the capabilities of wide bandgap semiconductors over silicon as power devices. Figures of Merit are used to better compare the possible device performance of these materials. Johnson’s Figure of Merit is a measure of the ultimate high frequency capability of the material. Baliga’s Figure of Merit is the measure of the specific on-resistance of the drift region on the vertical FET. The other Figures of Merit are name-explanatory (Tolbert 2003). In this table, the numbers have been normalized to Si, where larger numbers indicate better material/device performance. SiC and GaN have similar numbers, implying similar device performance, clearly out-performing Si in every category.

2.3.1 Silicon Carbide

SiC is the frontrunner in the research of wide bandgap semiconductor materials, making it the material for short wavelength optoelectronic, high temperature, high radiation, and high-
power/high-frequency electronic devices. SiC is capable of operating at high temperatures, emitting and detecting short wavelength light, making the fabrication of nearly solar blind UV imaging detectors possible.

SiC can withstand a voltage gradient (or electric field) over eight times greater than Si or GaAs without undergoing avalanche breakdown. This high breakdown electric field enables the fabrication of very high-voltage, high-power devices such as diodes, power transistors, power thyristors and surge suppressors, as well as high power microwave devices. Additionally, it allows the devices to be placed very close together, providing high device packing density for integrated circuits (Cree, 2006). Higher breakdown electric field also allows for thinner and more highly doped devices (Hornberger, 2004). SiC is an excellent thermal conductor, this enables SiC devices to operate at extremely high temperatures and still dissipate large amounts of heat (Cree, 2006).

SiC is a one-dimensional polymorphism called polytypism. An almost infinite number of SiC polytypes are possible, and approximately 200 polytypes have been discovered. Some of the more common polytypes include 3C, 2H, 4H, 6H, 8H, 9R, 10H, 14H, 15R, 19R, 20H, 21H, and 24R. SiC polytypes are differentiated by the stacking sequence of each tetrahedrally bonded SiC bi-layer. All of the polytypes form 1-D superlattice structures, except 2H and 3C. Electronic properties, such as effective mass, carrier mobility, and bandgap, vary widely between different polytypes of SiC.

Presently, two SiC polytypes are of interest in ongoing research: 4H-SiC and 6H-SiC. 6H-SiC has been the dominant polytype, but since 4H-SiC wafers were introduced in 1994, both have been
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used in research. Currently, 4H-SiC is preferred because the mobilities are identical along the vertical and horizontal planes of the semiconductor, which is not the case with 6H-SiC and its anisotropy (Tolbert, 2003).

Theoretical temperature dependencies of 4H-SiC and 6H-SiC are presented below, respectively. First, the theoretical temperature dependence of the bandgap for 4H-SiC and 6H-SiC (Goldberg, 2001), respectively:

\[ E_g = E_g(0) - 6.5 \times 10^{-4} \times \frac{T^2}{(T + 1300)} \]  \hspace{1cm} \text{Equation 3}

\[ E_g = E_g(0) - 6.5 \times 10^{-4} \times \frac{T^2}{(T + 1200)} \]  \hspace{1cm} \text{Equation 4}
Figure 13. Temperature dependence of the bandgap of 6H- and 4H-SiC.

Figure 13 illustrates the temperature dependence of 4H- and 6H-SiC bandgaps. As device temperature increases, the bandgap narrows. It is important to consider when modeling a material's performance over a temperature range.

2.3.2 Gallium Nitride

Although SiC has the longest history of all the wide bandgap semiconductors, GaN and other group III-nitrides have recently captured the spotlight. The group III-nitrides (AlN, GaN and InN) have direct band gaps which span the range 1.95-6.2 eV. They form a complete series of ternary alloys, which in principle make available any band gap within this range (Edgar, 1999). The wide bandgap offers a natural UV detector with very high, solar-blind DQEs. GaN detectors are compact, rugged, and can be fabricated radiation hard. They have very large LDRs (Joseph, 1999). The direct bandgap that group III-nitrides offer increases the optical transition probability by
Chapter 2. Theory

at least one order of magnitude compared to an indirect gap, such as SiC, for both absorption and emission of photons (Pankove, 1999). The group III-nitride materials also offer high breakdown voltage, and high peak electron velocity ($2.7 \times 10^7$ cm/s at room temperature) (Burm, 1999).

Presently, GaN substrates are not available. Progress in developing bulk GaN single crystals has been slow due to its inherent material characteristics. GaN is grown on foreign substrates where lattice and coefficient of thermal expansion (CTE) mismatches between the GaN epilayers and foreign substrate become problems. One approach involves growing a thick GaN epitaxial layer on a foreign substrate, after which the substrate is removed (Blevins, 2004). Two such substrates used are SiC and sapphire. SiC offers a good lattice match to GaN and also increases the total thermal conductivity of the material. However, since GaN is currently grown on SiC substrates, GaN's potential is limited by SiC wafer technology. In order to provide affordable GaN devices in the near future, it is important to develop other carrier wafer technologies, such as GaN on silicon, to make the GaN technology directly compatible with already established low cost industrial production methods (Wu, 2006).

It is known that GaN does not have good thermal conductivity, so utilizing SiC substrates (low lattice mismatch ~3%) in place of sapphire substrates for group III-nitride substrates, minimizes the self-heating effect of power devices due to the high thermal conductivity of SiC substrates (Burm, 1999).

GaN has two crystal structures, wurtzite and zinc blende. The majority of research on III-V nitrides has been focused on the wurtzite phase because the sapphire substrates transfer their hexagonal symmetry to the nitride film. Mizuta, et. al., first reported bulk zinc blende GaN grown on GaAs
surface in 1986. After that, interest in zinc blende nitrides intensified. It has been shown experimentally that zinc blende structure can be grown epitaxially (Li, Shuti, 2005).

The theoretical temperature dependence of wurtzite and zinc blende bandgap (Bougrov, 2001) is:

$$E_g = E_g(0) - 7.7 \times 10^{-4} \frac{T^2}{(T+600)}$$

Equation 5

Where $E_g(0) = 3.47$ eV for the wurtzite structure and $E_g(0)=3.28$ eV for the zinc blende.

Figure 14 illustrates the temperature dependence of zinc blende and wurtzite GaN bandgaps. As device temperature increases, the bandgap narrows.
2.4. Wide Bandgap Semiconductor Device Applications

Some potential imaging and non-imaging applications for wide bandgap semiconductors are listed below. Imaging detectors can be used in various fields particularly astronomy, industrial inspection, and medical imaging.

2.4.1 Imaging Applications

UV radiation is an integral part of the electromagnetic spectrum, just as are gamma-rays, x-rays, visible, IR and radio. Continued demand for UV observations with the Hubble Space Telescope and the results of several NASA-sponsored UV workshops suggest that continued exploration of the UV range will be essential for fundamental science in the foreseeable future (Ulmer, 1995). The topics that can be addressed cover aspects of astrophysics in fields from planetary science to cosmology:

- Planetary science: UV/FUV/EUV observations reveal auroral variability in planets, the dynamics of planetary upper atmospheres and cometary evaporation and gas production.

- Interstellar and intergalactic media: These are mainly studied through their absorption lines, superimposed on strong background sources, which appear exclusively in the UV/FUV and (in the case of helium) EUV.

- Stars: UV/FUV/EUV spectroscopy is essential for the study of hot star atmospheres, winds and evolution (including young neutron stars, white dwarfs, OB stars and Wolf-Rayet stars); cool star chromospheres, transition regions, coronae and winds; accretion and outflow physics in star formation and interacting binaries. This work can also be extended to the formation of massive stars and supernovae in external galaxies.
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- Cosmology: UV/FUV spectroscopy is essential for various cosmological observations including: the Gunn-Peterson effect for ionized helium, the cut-off energy in quasi-stellar objects, chemical evolution in active galactic nuclei and normal galaxies, high velocity clouds in active galactic nucleus (AGN), accretion rates and flows in massive central black holes, interaction between the radiation field and gas near central black holes, and the physics of star bursts from the Lyman continuum (Barstow, 2004).

In 2003, initial results using SiC for X-ray detection were published and following studies predicted SiC X-ray detectors could achieve remarkable performance at room or high temperature.

Bertuccio, et. al., presented experimental data on X-ray spectroscopy with SiC detectors for a wide temperature range that demonstrated the possibility to achieve high-energy resolution at room temperature with adequate resolutions up to 100°C. These results exposed two perspectives: (1) new applications involving x-ray detection or spectroscopy in harsh environments, (2) fabrication of X-ray spectrometers operating without any cooling equipment, which is generally necessary with systems employing other semiconductor detectors. This is a significant advantage for many applications because of the disadvantages previously described. A spectrometer employing SiC detectors can be very compact with low power consumption, useful for portable systems or for on-satellite spectrometers for X-ray astronomy (Bertuccio, 2004).

Another X-ray detector application can be found in Coordinate Measurement Machines (CMMs). The future of CMMs is non-destructive testing using X-ray technology with a new generation of Computer Tomography (CT). The promising new technology expands industrial tomography material inspection to accurate dimensional metrology, with applications to quality control and
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reverse engineering. Generally speaking, industrial CT involves the capture, processing and reconstruction of a 3-D work piece from multiple views to create an image of internal and external geometry (Hennessy, 2005).

Aside from industrial uses, CT is also used for medical purposes. CT became clinically available in the early 1970s. CT images are produced by passing x-rays through the body. An X-ray tube is rotated around the body and detectors, opposite the X-ray source, collect the transmission projection data. CT changed the practice of medicine by eliminating unnecessary exploratory surgery. Modern CT scans can detect cancer, ruptured discs, subdural hematomas, aneurysms, and a large number of other pathologies (Bushberg, 2002).

2.4.2 Non-imaging Applications

Most satellites and near-earth probes to date have used photovoltaic (PV) arrays for power generation. Missions probing closer to the sun, as illustrated in Figure 15, will require PV arrays that can function and withstand increased temperature, light intensity, and radiation. For example, the equilibrium temperature of a Mercury surface station will be about $450^\circ\text{C}$, much higher than current cells can handle.
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Figure 15. Artist's conception of proposed future mission to investigate the plasma environment near the sun (Landis, 2002).

It is desirable to develop approaches to high-temperature solar cell design that can operate under temperature extremes far greater than today's cells. Some of these design techniques can also reduce the cost and weight of solar arrays for other applications. Various techniques can be used; however the most promising application is to use wide bandgap semiconductors for the solar cells (Landis, 2002).

In the past decade, there has been a change of focus from gasoline and diesel engines to electric and hybrid electric vehicles. Increasing oil prices, pollution, concerns about a diminishing oil supply, and possible trade embargoes are creating a need for alternatives to these traditional vehicles. However, the present silicon technology is reaching the material's theoretical limits and cannot meet the requirements of the electric vehicles such as high temperature, high voltage and high current. Wide bandgap devices can function at higher temperatures and are smaller and
lighter than conventional semiconductor devices, resulting in a lighter vehicle; less load on the engine, faster acceleration and higher efficiency, finally resulting in less fuel or battery energy consumption (Ozpineci, 2006).

Alpha-voltaic batteries use a radioisotope, such as americium, as an energy source. These batteries offer a long life-time over conventional batteries. The radioisotope is coupled with a semiconductor device that operates like a solar cell to convert the alpha energy into electricity. The semiconductor device used needs to be able to withstand the harsh radiation conditions of the radioisotope alpha energy, such as a wide bandgap semiconductor. Research at Rochester Institute of Technology is developing alpha voltaic batteries that also have a buffer layer of radiation tolerant quantum dots placed on top of the semiconductor device (Bailey, 2005).

2.5 Fundamentals of Semiconductor Devices

2.5.1 P-N Junction

P-type (excess holes) and N-type (excess electrons) doped semiconductors are placed in contact with one another and the formed junction behaves differently than either type alone. Specifically, current will flow in only one direction (forward bias), creating a basic diode.
Figure 16 shows the schematic of a p-n junction. Diffusion causes the free electrons on the n-type side and free holes on the p-type side to initially wander across the junction. If a free electron meets with a free hole, they will recombine and be annihilated. As a result, there will be left a negative ion from the acceptor and a positive ion from the donor. Coulomb forces prevent further migration of the donors and acceptors across the junction. A space charge builds up creating a depletion region.
An applied voltage in the forward direction assists electrons in overcoming the coulomb barrier of the space charge in depletion region. Energy can be supplied to the free charge by an external voltage between the two ends of the p-n junction. (Colinge, 2002).

A large number of optoelectronic devices consist of p-n junction diodes. The key difference between these devices, such as photodiodes and solar cells, is their specific designs used to optimize light absorption, resulting in high energy-conversion efficiency.

When exposed to light, p-n junctions generate a photocurrent which opposes the diode current under forward bias. The diode can be used as a photodetector under reverse or zero bias voltage, as measured current is proportional to incident light intensity. The diode can be used as a solar cell under forward bias to generate electrical power.
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2.5.2 Charge Coupled Device

A charge-coupled device (CCD) is an array of metal-oxide-semiconductor (MOS) capacitors which can accumulate and store charge due to their capacitance. Figure 18 demonstrates a crude schematic of a single pixel of a buried channel CCD. The bulk material is p-silicon which can be made to have very small numbers of free electrons ("high resistivity") before exposure to light; this is important for best performance. An n-type channel is placed in contact to produce a p-n junction to create a depletion region where photo-generated electrons will be collected. Poly-silicon gates are grown on top of the insulating SiO2 with which the potential of the MOS capacitor is controlled. In Figure 18, there are three MOS capacitors per pixel, this is referred to as a three-phase CCD. It has the advantage of creating sub-pixel sensitivity.

Before exposure, the central electrode is set to a positive bias while the two neighboring electrodes are set negative. Setting the center electron positive further increases the potential in the silicon below that electrode where carriers are collected. The neighboring electrodes, with their lower potentials, act as potential barriers that define vertical boundaries of the pixel. Horizontal boundaries can be made with channel stops. When light of proper energy strikes the CCD surface, it frees electrons from the valence band to the conduction band where they accumulate in the capacitors. When the device is properly biased, freed electrons see a potential well (or depletion region) in which they can be trapped. The depletion region serves both to store photoelectrons and to shift them wholesale (Zimmerman, 2000).
Figure 18. One pixel of a CCD.
Chapter 3

Results

3.1 Theoretical P-N Junction Detector Efficiency

To date, the theoretical temperature dependence of p-n junction energy conversion efficiency has not been explored. Since p-n junctions are the basis of many optoelectronic devices, such as photodiodes, it is important to model their temperature dependences to verify that the best materials are being used that provide the best efficiency. While certain results are expected, this is the first time the actual physical equations have been examined with real semiconductor parameters. As efficiency limits are explored, the potential of wide bandgap semiconductors as harsh environment image detectors will be shown.
Chapter 3. Results

There are three basic parameters used to characterize performance and efficiency of a p-n junction device: (1) open circuit voltage (V_{OC}), (2) short circuit current (I_{SC}) (Green, 1982), and (3) the fill factor (FF) (Luque, 2003). Since the FF is a function of V_{OC}, only the ideal limits of I_{SC} and V_{OC} need to be examined in detail. Figure 19 illustrates the relationship between FF, I_{SC}, and V_{OC}.

![Figure 19. Three parameters of a p-n junction, I_{sc}, V_{oc}, and FF (Luque, 2003).](image)

For this analysis, the solar spectrum was chosen as the input power because of its well-studied and documented broad spectrum. To a good approximation, the sun acts as a perfect emitter of radiation as a black body. The resulting (average) energy flux incident on a unit area perpendicular to the beam outside the Earth's atmosphere is known as the solar constant, S = 1367 W/m². The extraterrestrial spectrum is denoted by AM0 (Luque, 2003). When the solar radiation enters the Earth's atmosphere, part of the incident energy is removed by scattering or absorption by air molecules, clouds, and aerosols. The total amount of radiation that reaches the ground is extremely variable.
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A concept, which characterizes the effect of a clear atmosphere on sunlight, is the air mass, equal to the relative length of the direct beam path through the atmosphere. On a clear summer day at sea level, the radiation from the sun at zenith corresponds to air mass 1 (AM1); at other times, the air mass is approximately equal to 1/cos $\theta$, where $\theta$ is the zenith angle. AM2 is the radiation of the early morning sun, just above the horizon. AM1.5 (Green, 1982) is the average of AM1 and AM2 and is the typical solar spectrum on the Earth's surface on a clear day, with total irradiance of 1 kW/m$^2$.

Using tables from Luque and Green which denote the irradiance values as a function of wavelength, the spectrums of AM0 and AM1.5, respectively were plotted in Figure 20.

![Figure 20. Solar spectrum for AM0 (Luque 2003) and AM1.5 (Green, 1982).](image-url)
Chapter 3. Results

Using the spectrums of AM0 and AM1.5, the short circuit current can be calculated. The short circuit current \( I_{sc} \) is the current flowing freely through the external circuit with no loaded resistance, in other words, the maximum current possible.

The upper limit of \( I_{sc} \) can be easily obtained for any semiconductor material. Under ideal conditions, each incident photon of energy greater than the bandgap energy generates one electron-hole pair. To calculate the maximum \( I_{sc} \) for these materials the photon flux of sunlight must be determined first. The photon flux is the irradiance per wavelength divided by the energy per individual photon of that wavelength, given by:

\[
F(\lambda) = \frac{W(\lambda)}{hc/\lambda}
\]

where \( W(\lambda) \) is the irradiance, \( h \) is Plank’s constant, \( c \) is the speed of light, and \( \lambda \) is the wavelength. Figure 21 shows the photon flux spectrum for AM0 and AM1.5. The calculated photon flux is in agreement with Green.
Chapter 3.  Results

The maximum $I_{sc}$ is calculated by integrating the photon flux from short wavelengths of energy greater than the bandgap up to the maximum wavelength that will generate electron-hole pairs within a particular semiconductor ($h\nu > E_g$). As an approximation to this definite integral, a numerical integral was taken using an average Riemann sum:

$$I_{sc} = \left(\frac{q}{2}\right) \left[ \sum_{n=0}^{n=N} (\lambda_n - \lambda_{(n-1)}) F(\lambda_{(n-1)}) \right] + \left(\frac{q}{2}\right) \left[ \sum_{n=0}^{n=N} (\lambda_n - \lambda_{(n-1)}) F(\lambda) \right]$$  

Equation 7

where $q$ is the charge of an electron. The result of the upper limit is seen in Figure 22. $I_{sc}$ is not dependent on temperature or materials. However, it is not surprising that as a semiconductor bandgap decreases with increased temperature, the short circuit current increases implying an indirect temperature dependence. As the bandgap decreases with increased temperature, the
energy of the photon required to generate electron-hole pairs decreases, shifting to longer wavelengths and in this case, allowing more of the solar spectrum to contribute to the photogenerated current. The calculated $I_{SC}$ is in agreement with Green.

![Graph](Figure 22. Limiting $I_{SC}$ for AM0 and AM1.5.)

The open-circuit voltage ($V_{oc}$) is the maximum voltage, or the voltage when the circuit is open and no current is flowing. For an ideal p-n junction, $V_{oc}$ is calculated as:

$$V_{oc} = \frac{kT}{q} \ln \left( \frac{I_s}{I_o} + 1 \right)$$

Equation 8
where $I_L$ is the light-generated current, $I_0$ is the diode saturation current, $k$ is Boltzmann's constant and $T$ is temperature. For this analysis the light-generated current is equal to the ideal short circuit current. The diode saturation current is expressed by:

$$I_0 = A(qD_e n_i^2 + qD_h n_i^2) = Aq\left(\frac{D_e}{L_e N_A} + \frac{D_h}{L_h N_D}\right)n_i^2$$

Equation 9

Where $A$ is the cross-sectional area, $q$ is the charge of an electron, $D_e$ and $D_h$ are the electron and hole diffusion coefficients, $n_i$ is the intrinsic concentration, $L_e$ and $L_h$ are the diffusion lengths for electrons and holes, $N_A$ and $N_D$ are the densities of acceptors and donors.

To maintain the maximum $V_{OC}$ thereby securing the maximum efficiency, $I_0$ needs to be as small as possible. One approach to calculating the upper limits of $V_{OC}$, suggested by Martin Green, is to assign favorable values to the semiconductor parameters in Equation 9 while keeping them within the range expected to produce reasonable devices.

The parameter that most strongly depends on semiconductor material choice is $n_i^2$; therefore the resulting approximation should have the same dependencies.

$$n_i^2 = N_c N_v e^{(-E_v/kT)}$$

Equation 10

The resulting estimation for a minimum $I_0$ as a function of bandgap and temperature is:
where $E_g$ is the bandgap energy. \[ I_o = 1.5 \times 10^5 e^{-E_g/kT} \]

Equation 11

ensures that the maximum $V_{oc}$ decreases with bandgap. This is opposite from what is observed for $I_{sc}$. Consequently this implies that there will be an optimum efficiency at a specific temperature.

The $V_{oc}$ decreases with increasing temperature, which can be seen from Figure 23, due to its dominating diode saturation current.

![Figure 23. Temperature dependence of $V_{oc}$ for AM0 and AM1.5.](image)

The fill factor is not as physically fundamental as $I_{sc}$ and $V_{oc}$. It represents the "squareness" of the IV curve of the p-n junction and describes the degree to which the voltage at the maximum power
Chapter 3. Results

Point \( V_{mp} \) matches \( V_{oc} \) and the current at the maximum power point \( I_{mp} \) matches \( I_{sc} \). It is a parameter having a value ranging from 0-1, with 1 being a square IV curve. For junctions of reasonable efficiency, the typical FF is between 0.7 and 0.85. For this analysis, a constant FF value within the range was used, 0.80.

An ideal fill factor that can be determined empirically using:

\[
FF = \frac{\frac{V_{oc}}{nRT/q} - \ln(V_{oc} + 0.72)}{V_{oc} + 1}
\]

Equation 12

where \( V_{oc} \) is the normalized \( V_{oc} \) defined as:

\[
V_{oc} = \frac{V_c}{(nRT/q)}
\]

Equation 13

where \( n \) is the ideality factor which typically ranges from 1 to 2 and is ideally equal to 1. The resulting FF is only valid for \( V_{oc} > 10 \) to about four significant digits.

Finally, employing all three of the fundamental parameters, the P-N junction energy-conversion efficiency is:

\[
\eta = \frac{P_{out}}{P_{in}} = \frac{V_{oc} I_{sc} FF}{P_{in}}
\]

Equation 14

where \( P_{in} \) is the incident power.
Chapter 3. Results

Figure 24. Efficiency as a function of bandgap for AM0 and AM1.5 at 300K. The solid lines use Equation 12 as the ideal FF and the dotted lines use a constant, “reasonable” FF of 0.8.

Figure 24 shows the maximum energy-conversion efficiency calculated as a function of bandgap. Using the AM0 spectrum as the input power, the peak efficiency is ~25% at a bandgap range of 1.3-1.6eV. The efficiency corresponding to Si is lower than the optimum efficiency seen here, at 1.4eV, which is the approximate bandgap of GaAs (gallium arsenide).

This efficiency was predicted in 1960 by Schockley and Queisser. They calculated the upper theoretical limit for the efficiency of p-n junction energy converters; a limiting efficiency, called the detailed balance limit of efficiency, in which the only recombination mechanism of hole-electron pairs is radiative. The efficiency is also calculated for the case in which radiative recombination is only a fixed fraction $f_c$ of the total recombination, the rest being nonradiative. Efficiencies were calculated with bandgap and $f_c$ as parameters, the sun and junction being assumed to be...
blackbodies with temperatures of 6000K and 300K, respectively. The maximum efficiency was found to be 30% for an energy gap of 1.1 eV and $f_c = 1$ (Shockley, 1961). The efficiency of Figure 24 matches Schockley and Queisser’s prediction.

3.2 Temperature Dependence of P-N Junction Efficiency

Figure 25 below shows detector efficiency as a function of bandgap over a temperature range of 50K through 1200K. Two observations can be made, first with increased temperature, overall efficiency decreases. Second, as the temperature increases there is a shift of the optimum efficiency per temperature to larger bandgaps. An optimal bandgap exists for a given operating temperature since the photon flux varies over photon energies, as also can be seen in Figure 25.

Figure 25. Theoretical AM0 performance as a function of bandgap for increasing temperature for FF=0.8.
Chapter 3. Results

The decreased efficiency as temperature increases is usually a result of a loss of open circuit voltage ($V_{oc}$), due to an increase in dark current (Mankins, 1997). As shown, the decrease in bandgap with increasing temperature provides a small increase in the short-circuit current ($I_{sc}$). However, any increase in $I_{sc}$ is generally offset by the more dominant decrease in $V_{oc}$.

3.3 Optimal-Efficiency Bandgap

Figure 26 aids in understanding why wide bandgap semiconductors provide optimum efficiency at higher temperatures. Simply put, as the temperature increases, the bandgap of the materials decreases. This allows more energy of the solar spectrum to impact the p-n junction. As it can be seen below, at 300K, 6H-SiC requires wavelengths less than 400nm to generate electron-hole pairs. As the temperature is increased and the bandgap decreases, this bandgap value shifts to the right, allowing more energy of the solar-spectrum to influence the p-n junction, generating electron-hole pairs. Concurrently, it is approaching the optimal efficiency bandgap value which is decreasing in value with increasing temperature. At some temperature they will intersect. At this temperature, 6H-SiC will have the optimum efficiency bandgap.
Chapter 3. Results

Figure 26. Solar Spectrum schematic of optimal efficiency bandgap and 6H-SiC bandgap. As the temperature increases, SiC bandgap approaches the optimal efficiency bandgap.

So far it has been shown that as temperature increases, the optimal efficiency shifts to wider bandgap semiconductors. A next step is to look at the efficiency of particular semiconductors over a large temperature range. Figure 27 shows the theoretical efficiency as a function of temperature for the wide-bandgap (GaP, SiC, and GaN) p-n junctions in comparison to a Si p-n junction. The effects of temperature on bandgap were taken into account for all semiconductors. The efficiencies decrease linearly with temperature as expected.

Figure 27 can be misleading. It shows the theoretical efficiencies for the materials listed not taking into account melting temperature, maximum p-n junction operating temperatures or any other parameters governing the physical performance of the device. As it can be seen, the color-coded vertical lines indicate the maximum operating temperature given by Chelnokov in Figure 7. This temperature is the temperature at which the p-n junction current is dominated by dark current and no longer controlled. As it can be seen, all semiconductors have theoretical working efficiencies
above their respective maximum operating temperature. It is always important to consider actual physical parameters when confirming theoretical results and conclusions.

![Diagram](image)

**Figure 27.** Theoretical efficiency for SiC, GaN, GaP, and Si p-n junctions as a function of temperature at AM0 and FF=0.80. Solid-vertical lines indicate the maximum operating temperature as stated from Chelnokov, 1997.

It appears from Figure 27, that GaP has the best efficiency of the wide bandgap semiconductors, followed by SiC and then GaN, up until temperatures of approximately 650K, the maximum operating temperature of GaP p-n junctions. GaN has the highest maximum operating temperature, at approximately 1260K with a theoretical efficiency of 3%.

A more concise way to look at these results can be seen in Figure 28 and Figure 29. As it has been stated previously, there exists a theoretical optimum efficiency per operating temperature and
Chapter 3. Results

an optimum-efficiency bandgap that gives that theoretical optimum efficiency per temperature. It was shown that this optimum-efficiency bandgap value increases with temperature.

\[ y = 1E-05x^2 - 0.0402x + 34.917 \]
\[ R^2 = 0.9999 \]

Figure 28. Optimum efficiency as a function of temperature for AM0 using FF=0.80.

\[ y = 1E-12x^4 - 3E-09x^3 + 3E-06x^2 + 2E-05x + 1.1228 \]
\[ R^2 = 0.9971 \]

Figure 29. Maximum bandgap (bandgap that gives the maximum efficiency) as a function of temperature for AM0 using FF=0.80.
Chapter 3. Results

Figure 28 extrapolates this data and shows in a continuous form the relationship of theoretical optimum efficiency as a function of temperature. As can be seen, it decreases to less than 5% at 1200K. Figure 29 shows the optimum efficiency bandgap as a function of temperature. The theoretical model shows a temperature of 1200K corresponds to an optimum-efficiency bandgap of approximately 2.3 eV.

Taking bandgap narrowing into account, 6H-SiC would have the theoretical optimum efficiency bandgap at approximately 1450K with a bandgap of approximately 2.50eV and an optimum efficiency of 1.96%, and GaN would have the optimum efficiency bandgap at approximately 1550K with a bandgap of approximately 2.60eV and an optimum efficiency of 1.34%. 4H-SiC would be the optimum efficiency bandgap at approximately 1600K with a bandgap of approximately 2.70eV and an optimum efficiency of 1.09%. While these temperatures are below the melting point of these materials, they are above the maximum operating temperature shown in Figure 7. However, the wide-bandgap junctions can function under higher temperatures with better efficiencies; they will be better able to handle the stresses of the high-temperature environment compared to the current detector materials due to inherent material properties.

Landis offers a theoretical approach to maximum operating temperature defined as the temperature at which the efficiency, extrapolated from the linear temperature coefficient, drops to zero, as seen in Figure 30 (Landis, 1994). While Si still remains about 470K, comparable with Chinook, SiC jumps to ~1500K.
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3.4 SUNS

In an effort to account for both temperature and light intensity, a theoretical relationship using Stephan-Boltzmann’s law was used. The initial relationship is found with AM0. The power per unit area of AM0 is known as the solar constant, \( S = 0.1367 \text{ W/cm}^2 \). The temperature associated with this intensity can be calculated by:

\[
T(x) = \left[ \frac{1}{\varepsilon \sigma} I \right]^{\frac{1}{4}}
\]

Equation 15
Chapter 3  Results

Where $\varepsilon$ is the emissivity and here equals 1, assumed to be a black body, and $\sigma$ is an experimental constant equal to $5.6705 \times 10^{-8}$ (W/m²K⁴). For AM0, the determined temperature is 394 K.

The following scaling law can be used to relate temperature and intensity:

$$XSuns = x \ast 0.1367 \left(\frac{W}{cm^2}\right)$$  \hspace{1cm} \text{Equation 16}

For the case where the p-n junction is in radiative equilibrium (i.e., under space conditions), the temperature will increase as the fourth root of the intensity according to the Stephan-Boltzmann laws. Table 3 shows the increase in temperature and intensity as a function of the number of Suns. Figure 31 shows the temperature and intensity dependence.

<table>
<thead>
<tr>
<th>Sun</th>
<th>Temp (K)</th>
<th>Intensity (W/m²)</th>
<th>Sun</th>
<th>Temp (K)</th>
<th>Intensity (W/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>701</td>
<td>13670</td>
<td>110</td>
<td>1276.129</td>
<td>150370</td>
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<tr>
<td>20</td>
<td>833</td>
<td>27340</td>
<td>120</td>
<td>1304.192</td>
<td>164040</td>
</tr>
<tr>
<td>30</td>
<td>922</td>
<td>41010</td>
<td>130</td>
<td>1330.553</td>
<td>177710</td>
</tr>
<tr>
<td>40</td>
<td>991</td>
<td>54680</td>
<td>140</td>
<td>1355.434</td>
<td>191380</td>
</tr>
<tr>
<td>50</td>
<td>1048</td>
<td>68350</td>
<td>150</td>
<td>1379.016</td>
<td>205050</td>
</tr>
<tr>
<td>60</td>
<td>1097</td>
<td>82020</td>
<td>160</td>
<td>1401.446</td>
<td>218720</td>
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<td>70</td>
<td>1140</td>
<td>95690</td>
<td>170</td>
<td>1422.848</td>
<td>232390</td>
</tr>
<tr>
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<td>1178</td>
<td>109360</td>
<td>180</td>
<td>1443.326</td>
<td>246060</td>
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<td>100</td>
<td>1246</td>
<td>136700</td>
<td>200</td>
<td>1481.849</td>
<td>273400</td>
</tr>
</tbody>
</table>

Table 3. The intensity and temperature for increasing SUN values.
Chapter 3. Results

Figure 3.1. Plot of the temperature and intensity dependence of Suns.

Finally, the power per unit area of a detector at XSuns is determined using Stephan-Boltzmann law:

\[
\frac{\text{Power}}{\text{Area}} \left( \frac{W}{cm^2} \right) = \varepsilon \cdot \sigma \cdot (T(XSuns))^4 - 3.2^4
\]

Equation 17

This equation takes into account the incident radiation and excitant radiation. The emissivity of SiC was based on Chawla's value of 0.8 (Chawla, 2003).

The efficiency as a function of Suns was determined. For this analysis, the same equation for efficiency was used, using \( P_m \) as the intensities shown in Table 4 with their corresponding temperatures. Also, the plots were completed taking the temperature dependence of the bandgap into account and determining the most accurate short circuit current for these bandgaps.
Chapter 3. Results

Figure 32. The temperature and intensity effects on efficiency as illustrated by Suns.

As the number of suns increases, the maximum efficiency decreases and shifts to wider bandgaps. Figure 33 shows the intersection of optimum efficiency bandgap and the bandgap of 6H-SiC as a function of SUNS. The intersection occurs at approximately 200 SUNS. This means that at 200 SUNS (1481.85 K, 273400 W/m²), 6H-SiC will have the optimum efficiency bandgap of approximately 2.5 eV. Again, this temperature is above the maximum operating temperature listed by Chelnokov. Figure 34 illustrates optimum efficiency as a function of SUNS. As can be seen, it decreases exponentially, and asymptotically approaches zero.
Chapter 3. Results

Figure 33. Intersection of optimum efficiency bandgap and the bandgap of 6H-SiC as a function of SUNS.

Figure 34. Optimal efficiency as a function of SUNS.
3.5 Experimental Efficiency of Wide Bandgap Semiconductor Devices

Experimental research conducted at Rochester Institute of Technology (RIT) compared the normalized efficiency as a function of temperature for p-n junctions of Si, InGaP, and SiC as shown in Figure 35. The slope of the least square fit to the data yield normalized temperature coefficients of -4.6 and -1.6 for the Si and InGaP cells, respectively. These are in good agreement with comparable values reported in the literature. In contrast, SiC has a positive temperature coefficient. SiC was the only junction that was still functional above 400°C (673K), and it actually had a slightly improved efficiency over its room temperature value. This is a very important discovery, as it confirms the theoretical results and has not yet been shown in the literature. In the end, this result is expected considering its 3.0 eV bandgap is beyond the peak in the solar spectrum, as shown in Figure 26, therefore its short circuit current benefits greatly from any bandgap narrowing which dominates the efficiency.
Figure 35. Normalized efficiency of InGaP and SiC to Si as a function of temperature.
Chapter 4

Conclusions and Future Work

While narrow bandgap semiconductors offer the best efficiencies at lower temperatures of general use, the operation of devices at high temperature and radiation conditions requires development of wide-bandgap materials and devices. The optimum bandgap of a device as a function of temperature was determined, and shows that the bandgap increases from slightly less than 1.5 eV from 300 K, to about 2 eV for operation at 1000 K, and even further, about 3 eV for operation at 2000K.
Chapter 4. Conclusions and Future Work

A test conducted on p-n junctions of Si, InGaP, and SiC at Rochester Institute of Technology provided an initial confirmation of the theoretical results. The experimental results showed that SiC was the only one of the junctions to have a positive temperature coefficient and as a result, dominated the efficiency at higher temperatures as expected.

This data proves the potential for wide bandgap semiconductors as detector materials in high temperature, high intensity, and hence harsh environments. Even though wide bandgap semiconductors have low efficiency at low and room temperatures, they dominate p-n junction efficiency at higher temperatures as their bandgaps approach the optimal bandgap for maximum efficiency.

Future work would entail confirming the maximum operating temperature determined experimentally by Chelnokov and theoretically by Landis for p-n junctions of interest, such as SiC and GaN. These temperatures would be confirmed for both biasing modes of the junction, forward and reverse.
Appendix

A.1 Fundamentals of Semiconductors

A.1.1 Crystal Structure

All solid materials are classified by the manner in which their atoms are arranged. Semiconductors are crystalline solids with highly ordered atoms that are categorized by their crystal structure and underlying lattice. The lattice is generated by three unit vectors, \( a_1, a_2, \) and \( a_3 \) and a set of integers, \( k, l, \) and \( m \) so that each lattice point can be reached by vector, \( \vec{r} \):

\[
\vec{r} = k\vec{a}_1 + l\vec{a}_2 + m\vec{a}_3
\]
Appendix A

The construction of the lattice point from the set of unit vectors is shown in Figure A. 1, where $k=3$ and $l=2$.

![Figure A. 1. The construction of lattice points using unit vectors.](image)

Cubic lattices are common semiconductor lattices. The three cubic lattices are simple cubic, body-centered cubic, and face-centered cubic, as shown in Figure A. 2. All unit vectors identifying the traditional unit cell have the same size; the crystal structure is completely defined by a single number, the lattice constant, $a$.

![Figure A. 2. Three cubic lattices: (a) simple cubic, (b) body-centered cubic, and (c) face-centered cubic.](image)
Appendix A

More specifically, the most common crystal structure found in semiconductors is the diamond lattice as seen in Figure A.3. Each atom in the diamond lattice has a covalent bond with four adjacent atoms, which altogether form a tetrahedron. This lattice can also be formed from two face-centered cubic lattices, which are displaced along the body diagonal of the larger cube by one quarter of that body diagonal.

![Diamond lattice structure]

Figure A.3. Diamond structure of silicon and germanium

Compound semiconductors, such as gallium arsenide (GaAs), have crystal structures similar to a diamond structure. Each atom still has four covalent bonds, but they are bonds with atoms of the different material. This structure is referred to as the zinc-blende lattice named after zinc-sulfide (ZnS). A third common structure is the hexagonal structure also called the wurtzite crystal structure. Hexagonal crystal structures are characterized by the lattice constant, a, and c, the distance between the hexagonal planes.
Figure A. 4. Cubic unit cell for the zinc-blende structure. The face centered cubic has a basis of two different atoms represented by the open and solid spheres (Razeghi, 2002).

Figure A. 5. Hexagonal crystal structure (Sah, 1991).

Many semiconductors have more than one crystal structure. GaAs, GaN, and SiC are a few that can either be cubic or hexagonal (Luque, 2003).

A.1.2 Energy bands

Semiconductors have energy bands consisting of a large number of closely spaced energy levels. The bands can be thought of as the collection of the individual energy levels of electrons surrounding each atom. The wave functions of individual electrons overlap with electrons of
neighboring atoms. However, the Pauli Exclusion Principle does not allow electron energy levels to be the same so instead a set of closely spaced energy levels forms an energy band. The electrons in the top and bottom of such a band behave similarly to free electrons, as in metals. However, semiconductors are physically different than metals so an adjustment is introduced to the mass of the electron to account for this. This is referred to as the effective mass.

Energy band diagrams for semiconductors can be simplified since only the electrons in the highest almost-filled valence band and the lowest-almost empty conduction band dominate behavior. The energy separating the valence and conduction bands is known as the “forbidden” energy bandgap.

Figure A. 6 shows a basic schematic of semiconductor energy bands. The top band indicates the conduction band, $E_c$. The bottom band is the valence band, $E_v$. The energy bandgap, $E_g$, is located between these two bands.

An important feature of the energy band diagram is whether or not the minimum conduction band and maximum valence band occur at the same value of the wave number. If they do, the energy bandgap is direct. If not, it is indirect (Green, 1982). Figure 12 illustrates direct and indirect
Appendix A

bandgaps (adapted from Singh, 2005). This is an important distinction as direct bandgaps provide more efficient light absorption and emission. As it can be seen in Figure A. 7, Si has an indirect bandgap while GaAs has a direct bandgap (Simmons, 2000).

![Diagram of indirect and direct bandgaps]

Figure A. 7. Schematic of indirect and direct bandgaps. The direct bandgap conduction band is illustrated with the solid line and the conduction band of the indirect bandgap is the dashed line (adapted from Singh, 2005).

![Diagram of GaAs and Si band structures]

Figure A. 8. Sketch of the band structures of GaAs (direct) and Si (indirect) (Simmons, 2000).
Appendix A

The bandgap of a semiconductor can be altered by temperature. As the thermal energy of the semiconductor increases, the amplitude of the atomic vibrations increases, resulting in the increase of the interatomic spacing. This decreases the average potential seen by the electrons in the materials, which reduces the energy bandgap. A direct modulation of the interatomic distance, such as compressive or tensile stress can affect the bandgap as well.

The temperature dependence of the energy bandgap has been experimentally determined yielding:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$  \hspace{1cm} \text{(A.2)}

Doping the semiconductor with impurities also affects the bandgap. The wave functions of the electrons bound to the impurity atoms start to overlap as the density of the impurities increases. This overlap forces the energies to form an energy band, rather than a discreet level, thereby decreasing the conduction and valence band energy difference. More on impurities will be explained later.

If the impurity level is shallow, the impurity band reduces the energy band of the host material by:

$$\Delta E_g(N) = \frac{-3q^2}{16\pi\varepsilon_s} \sqrt{\frac{q^2N}{\varepsilon_s kT}}$$  \hspace{1cm} \text{(A.3)}

where \(N\) is the doping density, \(q\) is the charge of an electron, \(\varepsilon_s\) is the dielectric constant of the semiconductor, \(k\) is Boltzmann's constant and \(T\) is the temperature.
A.1.3 Impurity and Donor/Acceptor Atoms

Impurity atoms can exist in a crystal in two ways: (1) interstitial impurities: atoms occupy positions squeezed in between host atoms, and (2) substitution impurities: substitute a host atom maintaining the regular atomic arrangement in the crystal. Impurities happen unintentionally as described by interstitial impurities, as a result of poor crystal growth quality or intentionally, with substitution impurities, with a process called doping. Doping semiconductors changes the inherent properties of the host semiconductor, with the aim of alerting them for a specific use.

Semiconductors can be doped by either a p-type or n-type impurity atom. A p-type impurity atom will provide an excess of holes. N-type impurity atoms will provide an excess of electrons.

If considering a covalent bond in the valence band, four valence host electrons are used, but a fifth electron of an n-type substitution impurity atom is in a different situation. It is not in the covalent bond, therefore not in the valence band. However, it is still tied to the valence band substitution atom. The extra electron lies at energy $E_i'$ below the edge of the conduction band. This places an allowed energy level within the forbidden bandgap.

If a p-type substitution atom is considered, this material does not have enough valence electrons to satisfy four covalent bonds. This gives rise to a hole tied to the substitution atom in the conduction band. Hence, the substitution atom in the conduction band gives rise to an allowed energy level for electrons in the bandgap just above the valence band. Figure A. 9 illustrates these new energy levels.
Appendix A

Figure A. 9. (a) Energy of the allowed state introduced into the bandgap by a valence band substitution impurity. (b) Corresponding energy state for a conduction band substitution impurity (Green, 1982).

Since the energy to release the extra electron in the valence band is small; most of the impurity electrons have acquired enough energy at room temperature and jumped to the conduction band. As a result, most substitution n-type atoms in the valence band have a positive net charge. These n-type substitution atoms are known as donors.

The total number of electrons in conduction band and holes in the valence band in this case can be found by considering the condition for charge neutrality in semiconductors:

\[ p - n + N_{D}^{+} = 0 \]  \hspace{1cm} A 4

Where \( p \) is the hole density in the valence band, \( n \) is the density of electrons in the conduction band, and \( N_{D}^{+} \) is the density of ionized donors. Since the vast majority of donors will be ionized, \( N_{D}^{+} \) will be nearly equal to the total density of donors, \( N_{D} \). From Equation 4, \( n \) will be greater than \( p \) and very much greater when \( N_{D} \) becomes large. Therefore, the approximations come out to:
Similarly, the p-type substitution atom can easily give up excess holes to the valence band or equivalently accept electrons. They are known as acceptors; they "accept" electrons. An ionized acceptor has a negative net charge, hence (Green, 1982):

\[ p - n - N_A^- = 0 \]  

\[ N_A^- \approx N_A \]  

\[ p \approx N_A \]  

\[ n \approx \frac{n^2}{N_A} \ll p \]
A.1.4 Carrier Distribution Function

At low temperatures, electrons in a semiconductor occupy the lowest possible energy states. However, all electrons cannot occupy the very lowest allowed energy level due to the Pauli Exclusion Principle. Therefore, at low temperatures all available states in the semiconductor up to a certain energy level, the Fermi level, $E_F$, will be occupied by two electrons of opposite spin.

As temperature increases some electrons gain energy in excess of $E_F$. The probability of occupation of an allowed energy state of any given energy, $E$, can be calculated from statistical consideration for this general case. The result is the Fermi-Dirac distribution function also known as the Fermi Function.

The system is characterized by its temperature, $T$, and its Fermi energy, $E_F$. Therefore, the Fermi function is:

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}}$$  \hspace{1cm} \text{(A12)}

Figure A. 10 exhibits the Fermi Function at increasing temperatures from 150K to 600K. As the temperature increases, the positive difference between the given energy, $E$, and the Fermi energy, $E_F$, increases. This leads to an increase in the probability of occupancy of the given energy levels by electrons (Luque, 2003).
Appendix A

Figure A. 10. The Fermi function at T=600K, 300K, and 150K.

A.1.5 Density of States

The density of states is of interest because it allows the determination of the density of carriers. Once the number of available states at each energy level is known, the number of electrons at each energy level can be obtained.

The density of states in a semiconductor equals the density per unit volume per unit energy of the number of solutions to Schrödinger's equation. For simplicity, it will be assumed that the semiconductor can be modeled as an infinite quantum well where electrons, with effective mass, $m_e^*$, are free to move. The semiconductor is assumed to be a cube with length, $L$. The solutions to the wave equation are sine and cosine functions. The wave function must be zero at the infinite...
Appendix A

barriers of the well; \(x=0\) and \(x=L\). The coefficients of the solution are to be determined based on initial conditions.

The density per unit energy is obtained by:

\[
\frac{dN}{dE} = \left( \frac{L}{\pi} \right)^3 \pi k^2 \frac{dk}{dE}
\]

And the density of states per unit volume per unit energy is:

\[
g(E) = \left( \frac{1}{L^3} \right) \frac{dN}{dE} = \frac{8\pi \sqrt{2}}{h^3} m^* \frac{3}{2} \sqrt{E}
\]

for \(E \geq 0\). The minimum energy of the electron is the energy at the bottom of the conduction band, \(E_c\), so that the density of states for electron in the conduction band is given by:

\[
g_e(E) = \frac{1}{L^3} \frac{dN}{dE} = \frac{8\pi \sqrt{2}}{h^3} m_e \frac{3}{2} \sqrt{(E - E_c)}
\]

For \(E \geq E_c\) for the energy of an electron. The density of states for holes in the valence band is given by:

\[
g_v(E) = \frac{8\pi \sqrt{2}}{h^3} m_h \frac{3}{2} \sqrt{(E_v - E)}
\]
Appendix A

For $E \leq E_v$ for the energy of a hole (Yu, 2001).

### A.1.6 Carrier Densities

The density of electrons in a semiconductor is related to the density of available states and the probability that each of these states is occupied. Due to the nature of the Fermi function, most of the electrons in the conduction band and holes in the valence band are clustered near the band edges. The total number in either band can be found by performing integration. The number of electrons in the conduction band per unit volume of the semiconductor, $n$, is given by:

$$n = \int_{E_v}^{E_c} f(E) g_c(E) dE$$  \hspace{1cm} (A17)

The final result of integration is:

$$n = N_c e^{(E_v - E_c)/kT}$$  \hspace{1cm} (A18)

Where $N_c$ is a constant at fixed temperatures, known as the effective density of states in the conduction band.

$$N_c = 2 \left( \frac{2\pi m_e^* kT}{\hbar^2} \right)^{3/2}$$  \hspace{1cm} (A19)
Appendix A

Similarly, the total number of holes in the valence band per unit volume of the crystal is given by:

\[ p = N_v e^{(E_v - E_f)/kT} \]  \hspace{1cm} \text{(A 20)}

Where \( N_v \) is similarly defined and known as the effective density of states in the valence band.

Both \( N_c \) and \( N_v \) are constant values at fixed temperatures.

For the idealized case of a pure and perfect semiconductor without surfaces, \( n \) equals \( p \) because each electron in the conduction band leaves a hole in the valence band. Hence:

\[ n = p = n_i \]  \hspace{1cm} \text{(A 21)}

\[ np = n_i^2 = N_c N_v e^{(E_v - E_f)/kT} \]  \hspace{1cm} \text{(A 22)}

\[ n_i^2 = N_c N_v e^{(-E_f)/kT} \]  \hspace{1cm} \text{(A 23)}

Where \( n_i \) is the intrinsic carrier concentration. Also because \( n = p \), the Fermi energy can be written as:

\[ E_F = \frac{E_v + E_f}{2} + \frac{kT}{2} \ln \left( \frac{N_v}{N_c} \right) \]  \hspace{1cm} \text{(A 24)}
Appendix A

Therefore, the Fermi level in a pure and perfect semiconductor lies close to mid-gap, being offset only by differences in the effective density of states in the conduction and valence bands (Green, 1982).

A.1.7 Carrier Transport

Movement of free carriers leads to current in a semiconductor. Carrier motion can be caused by an electric field due to an externally applied voltage, otherwise known as carrier drift, as shown in Figure A. 11. Carriers also move from regions of high carrier density to regions of low carrier density; this motion is due to thermal energy and the random motion of carriers, otherwise known as carrier diffusion. The total current is equal to the sum of the drift and diffusion currents.

![Electron drift in a semiconductor caused by an applied electric field. Electron travels with velocity, v.](image)

As an electric field is applied, the electrostatic force causes the electrons (carriers) to first accelerate in the direction opposite to the field and holes in the direction of the field. Due to collisions with impurities and lattice vibrations, the electron motion becomes randomized and reaches an average drift velocity, v:
Appendix A

\[ v_d = \frac{1}{2} \alpha t = \frac{1}{2} \frac{q t_r}{m_e^*} E \]  
A 25

for electrons in the conduction band, where E is the electric field, \( t_r \) is the relaxation time of the electron, \( m_e^* \) is the effective mass of the electron and \( q \) is the charge of an electron. The ratio of the velocity to the applied field is called the mobility:

\[ \mu = \frac{|v|}{|E|} = \frac{q t_r}{m^*} \]  
A 26

Both holes and electrons have different mobilities due to their respective relaxation times and effective masses. The corresponding current flow due to conduction band drift electrons will be:

\[ \bar{J}_e = q n \mu_e \bar{E} \]  
A 27

A similar equation for holes in the valence band:

\[ \bar{J}_h = q p \mu_h \bar{E} \]  
A 28

Diffusion of carriers exists when there is a carrier density gradient. This can be made by varying the doping densities or by applying a thermal gradient. Since current is proportional to the flux of charged particles, the current density corresponding to a one-dimensional concentration gradient of electrons is:
Appendix A

\[ J_e = qD_e \frac{dn}{dx} \]  
A 29

Where \( D_e \) is the diffusion constant. For holes:

\[ J_h = -qD_h \frac{dn}{dx} \]  
A 30

Drift and diffusion processes are fundamentally related through the mobility and the diffusion constant:

\[ D_e = \frac{kT}{q} \mu_e \]  
A 31

\[ D_h = \frac{kT}{q} \mu_h \]  
A 32

The total electron current in a semiconductor is the diffusion current added to the drift current:

\[ J_n = qn\mu_n E + qD_n \frac{dn}{dx} \]  
A 33

And for holes:

\[ J_p = qp\mu_p E - qD_p \frac{dp}{dx} \]  
A 34
The total current is therefore the sum of the electron and hole current densities multiplied by the area, $A$, perpendicular to the direction of the carrier flow:

$$ I = A(J_n + J_p) $$

Both drift and diffusion currents experience scattering due to collisions. For pure semiconductors of good crystalline quality, the collisions that randomize the carrier velocities will involve the atoms of the host crystal. However, ionized dopants are very effective scatters because of their associated net charge. Consequently, as the semiconductor becomes more heavily doped, the average time between collisions decreases therefore mobility decreases. Less specialized impurities as well as crystal defects will decrease mobilities further, for similar reasons.

Increasing temperatures will increase the vibration of the host atoms, making them larger collision “targets”, also decreasing the average time between collisions and carrier mobilities. This effect becomes less pronounced at high doping levels, where ionized dopants are the more dominate effective carrier scatterers.

Increasing the strength of the electric field will eventually increase the drift velocities of carriers to values where they will become comparable to the random thermal velocities. Hence, the total velocity of electrons will ultimately increase with field strength.
Appendix A

The conductivity of a material is defined as the current density divided by the applied electric field. The current density can be expressed as a function of electric field using mobility:

\[ J = qnv_e + qpv_h = q(n\mu_e + p\mu_h)E \]  

So the conductivity due to electrons and holes is (Luque, 2003) (Green, 1982):

\[ \sigma = \frac{J}{E} = q(n\mu_e + p\mu_h) \]

A.1.8 Thermal Conductivity

At elevated temperatures, or in extreme self-heating circumstances, proper heat dissipation is essential. A temperature increase due to the self-heating of an operating device is inversely proportional to the thermal conductivity (Burm, 1999).

The rate of thermal transport within a material is governed by the thermal diffusivity, which is the ratio of the thermal conductivity to the heat capacity. The heat capacity is defined as the change in internal energy of a material resulting from a change in temperature. The energy within a crystalline material, which is a function of temperature, is stored in the free electrons of a metal and within the lattice in the form of vibrational energy (Bejan, 2003).
A.1.9 Carrier Recombination and Generation

Fundamental absorption refers to the annihilation or absorption of photons by the excitation of an electron from the valence band to the conduction band, leaving behind a hole in the valence band. Intensity of radiation, $I(x)$, at a depth, $x$, within a solid is given by Lambert-Beers Law:

$$I(x) = I_0 \exp(-\alpha x)$$

Where $I_0$ is the incident radiation intensity and $\alpha$ is the absorption coefficient at a wavelength, $\lambda$, and absorption depth, $d \approx 1/\alpha$ (Jha, 1995). Photons with energy greater than the bandgap generate electron-hole pairs with a rate proportional to the linear absorption coefficient of the materials and to the local incident intensity. The light intensity decays rapidly with increased distance traveled within material (Pearson, 2000). Photons with energy less than $E_g$ cannot be absorbed and the semiconductor is considered transparent for these photons.

As stated, the absorption coefficient strongly depends on wavelength. For wavelengths with energy larger than the bandgap energy, the absorption coefficient increases rapidly according to the so-called fundamental absorption. The steepness of the onset of absorption depends on the kind of band-to-band transition: direct bandgaps have a steep onset and indirect bandgaps have a shallow onset (Zimmerman, 2004).
Appendix A

Both energy, \( E \), and momentum, \( p \), must be conserved in such a transition. A photon has large energy but small momentum. For the case of a direct bandgap semiconductor, because the photon momentum is small compared to the existing crystal momentum, the latter is essentially conserved in the transition. The energy difference between the initial and final state is equal to the energy of the original photon:

\[
E_f - E_i = hf
\]

A 39

In terms of parabolic bands:

\[
E_f - E_c = \frac{p^2}{2m_e^*}
\]

A 40

\[
E_v - E_v = \frac{p^2}{2m_h^*}
\]

A 41

Leading to the specific crystal momentum at which transition occurs:

\[
hf - E_g = \frac{p^2}{2} \left( \frac{1}{m_e^*} + \frac{1}{m_h^*} \right)
\]

A 42

As the photon energy increases the value of crystal momentum at transition also increases. The energy away from the band edge of both initial and final states also increased. The probability of absorption depends on the density of electrons at the energy corresponding to the initial state and
the density of empty states at the final energy. Since both these quantities increase with energy away from the band edge, it is not surprising that the absorption coefficient increases rapidly with increases photon energy above $E_g$. A theoretical result gives:

$$\alpha(h\nu) \approx A^* (h\nu - E_g)^{1/2}$$

Where $A^*$ is a constant equal to $2 \times 10^4$ when $\alpha$ is in units of cm$^{-1}$ and $h\nu$, the energy of the photon, and $E_g$ are in units of eV.

Since light intensity drops to $1/e$ of its value in passing a distance $1/\alpha$ through the semiconductor, Equation A 43 shows that radiation of photon energy greater than $E_g$ is absorbed within the first few microns of entering a direct bandgap semiconductor (Green, 1982).

In some semiconductors, quantum selection rules do not allow transitions at $p=0$ but allow them for $p \neq 0$. In such cases:

$$\alpha(h\nu) \approx \frac{B^*}{h\nu} (h\nu - E_g)^{1/2}$$

Where $B^*$ is a constant (Luque, 2003).

In the case of an indirect bandgap semiconductor, the minimum energy in the conduction band and maximum energy in the valence band occur at different crystal momentums. Photon energies
Appendix A

much larger than the forbidden gap are required to give direct transitions of electrons from the valence to conduction band.

However, transitions can occur at lower energies by a two-step process involving photons and phonons. An electron can make the transition from the maximum energy in the valence band to the minimum energy in the conduction band in the presence of photons of suitable energy by emission or absorption of a phonon of the required momentum. Hence the minimum photon energy required to excite an electron from the valence band to conduction band is:

$$h\nu = E_g - E_p$$  \hspace{1cm} \text{(A 45)}$$

Where $E_p$ is the energy of the absorbed phonon with required momentum. Since indirect bandgap semiconductor absorption process requires that an extra "particle" be involved, the probability of light absorption by this process is much less than direct bandgap semiconductors. Therefore, the absorption coefficient is low and light can pass a reasonable distance into the semiconductor before absorption. The theoretical absorption coefficient for indirect bandgap semiconductors is:

$$\alpha_\nu(h\nu) \approx \frac{A(h\nu - E_g + E_p)^2}{\exp \left[\frac{E_p}{kT}\right] - 1}$$  \hspace{1cm} \text{(A 46)}$$

For a transition involving phonon emission:
Since both phonon emission and absorption are possible for $hf > E_g + E_p$, the absorption coefficient is then:

$$\alpha_e(hf) \approx \frac{A(hf - E_g - E_p)^2}{1 - \exp \left[ - \frac{E_p}{kT} \right]}$$  \hspace{1cm} \text{(A 47)}$$

The photon is absorbed in this process and the excess energy, $E_{ph} - E_g$, is added to the electron and the hole in the form of kinetic energy (Green, 1982).

Free carrier absorption, where an electron in the conduction band absorbs energy of a photon and moves to an empty state higher in the conduction band is typically only significant for photons with energy, $E < E_g$. It can be ignored in single p-n junctions because it does not affect creation of electron hole pairs (Luque, 2003).

Recombination occurs when holes and electrons annihilate each other. An electron occupies an empty state, and both carriers disappear. The energy difference between the initial and final state of the electron is released in the process. There are different types of recombination: (1) band-to-band, (2) trap-assisted, and (3) auger recombination. Band-to-band recombination occurs when an electron moves from its conduction band into an empty valence band level associated with a hole. This transition is commonly also a radiative transition in direct bandgap semiconductors. Radiative recombination emits this energy in the form a photon (Green, 1982).
A.2 CCD Charge Transfer

CCD arrays are read-out by transferring the charge from one MOS capacitor to its neighbor. This is done by clocking the gate voltages. In a typical CCD, a three-phase array is used where each pixel has three gate electrodes, as shown in Figure A. 12. In each row of pixels, the corresponding electrodes on each pixel are connected. The parallel shift registers are shown as rows running across the whole face of the CCD. These can be separated by insulating channel stops preventing electron bleed from neighboring pixels. At one end is a column of serial shift electronics and an output amplifier. Good performance depends on near-100% transfer of the electrons to/from each electrode with no smearing or generation of spurious electrons. Each parallel transfer places the contents of one pixel in each row into the serial register column. This column is then shifted out vertically through the output amplifier and into memory before the next parallel transfer occurs (Waynant, 2000).
Figure A. 12. This image shows the sequence, from top to bottom, of the principle of charge transfer in a CCD: charges are moved to the output amplifier by changing the electrode voltages (Bely, 2003).

CTE or charge transfer efficiency is a measure of how well the charge transfer was completed. A value of 1 is perfect CTE. By today’s standards, CTEs of 0.99999 are expected per transfer. CTE is determined through a procedure using x-rays where it is known very accurately that one 5-keV x-ray photon produces 1620 electrons.

As a measure of detector capabilities, it is typically calculated for the “worst” pixel location or the pixel location that has to go through the most transfers before it is read out. If a 10x10 pixel CCD is being read out, the final CTE of the “worst” case pixel would be \((0.99999)^{100} = 0.999\) which is considered a good CTE. However, as CCDs get larger, the “worst” case pixel experiences decreasing CTEs. If a 100x100 CCD is considered, the “worst” case pixel would have a final CTE of \((0.99999)^{10000} = 0.9048\). This is not considered a good value. This becomes a problem for larger CCDs. CTE can be affected by incomplete transfers, (simply meaning that there was not enough...
time to transfer the electrons), surface state trapping, bulk trapping, and inter-electrode gap trapping. Buried channel CCDs reduce surface state trapping and have better CTEs.

A.3 Current Industrial Status of SiC and GaN

First and foremost, the bulk crystal growth method of wide bandgap semiconductors is different from conventional growth methods. Extremely high temperatures and pressures are necessary to melt these materials. Instead, a vapor or epitaxial type of growth is required. These processes create new challenges with respect to controlling thermal gradients, impurities, and defect generation. Many in the industry also mention a need for the ease in the transition from Si wafer and device production to wide bandgap semiconductor wafer and device production. As mentioned above, since different growth techniques are required for wide bandgap semiconductors, current Si “machinery” and technology cannot be used and therefore, there is a lag in the ability to speed up commercialization of wide bandgap semiconductor wafers because the infrastructure does not yet exist (Blevins, 2004).

The SiC electronic device market will be worth over $50 million by 2009 according to a report by German market analyst Wicht Technologie Consulting (WTC). Although almost 80% of SiC substrates will be used for high-brightness blue, green and white LED manufacture, “fresh” markets will emerge for a new generation of energy-efficient, high-performance diodes and transistors used in power supplies and electric motors.
Appendix A

The company predicts that the global market for SiC Schottky diodes and transistors will increase from $13 million in 2004 to more than $53 million in 2009. The market for replacement power supplies that could contain SiC diodes is worth several billion dollars. If these devices were used in conjunction with SiC MOSFETs, then ten-fold improvements in energy savings would be possible.

Today’s SiC Schottky diode market is headed by the US Company Cree, which holds a market share of 50%, and Germany-based Infineon. Cree also has a 95% share of the far smaller and less mature transistor market. Rockwell Scientific is the only other commercial supplier of SiC MESFETs. WTC also expects Cree’s dominance in the SiC substrate market to continue.

However, it added that the Finland-based Norstel, which also sells SiC substrates, will take a significant share of the relatively small European market for power device substrates.

Since 2000, GaN research activities have intensified around the world. The number of companies and research centers with GaN activity has increased to over 500 organizations in early 2005 from roughly 350 such organizations identified in 2000.

Blue, green, and white LED technology has continued its large-scale commercial growth resulting in revenues exceeding $3 billion in 2004. White LEDs are responsible for over 50% of the total GaN related LED market. Future high-growth GaN devices include high-power LEDs for lighting, deep UV emitters, and laser diodes. The latter will be used in the next generation of optical storage technology and their development will be spurred by increasing availability of GaN substrates (CompoundSemiconductor.net, 2005).
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