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Cold X-ray Effects on Satellite Solar Panels in Orbit

By

Myles Fogleman

Thesis

Submitted for the fulfilment of

Master Degree in Nuclear and Mechanical Engineering

Virginia Commonwealth University

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Advisor:

Dr. Gennady Miloshevsky

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Abstract

An exo-atmospheric nuclear detonation releases up to 80 percent of its' energy as X-rays. Satellite's solar cells and their protective coatings are vulnerable to low energy X-ray radiation. Cold X-rays (~1-1.5 keV) are absorbed close to the surface of materials causing the blow-off and rapid formation of Warm Dense Plasmas (WDPs), particularly in a gap between the unshielded active elements of solar cells. To understand how WDPs are created, it is necessary to investigate the power density distribution produced by cold X-rays for typical solar panel surface materials. The Monte Carlo stepping model implemented in the GEANT4 software toolkit is utilized to determine the power density created by cold X-rays in a multi-layered target composed of a layer of an active cell shielded by layers of cover glass and anti-reflective coating. The power density generated by cold X-rays in the unshielded semiconductor layer at different incidence angles is also investigated in order to account for different orientations of the satellite's solar panels with respect to the point of nuclear detonation. The flux spectrum of X-rays originating from a nuclear blast is described by the Planck's blackbody function with the temperature from 0.1 keV to 10 keV. The secondary radiation (photo-electrons, fluorescence photons, Auger- and Compton-electrons) resulting from absorption and scattering of primary X-rays is taken into account in the redistribution of energy deposition within slabs. The profiles of power density within the slab system produced by primary cold X-rays, secondary photons and electrons are calculated as a function of depth. The discontinuity in power density profiles is observed at the interfaces of slabs due to discrete changes in stopping power between slab materials. The power density is found to be higher in slab materials with higher mass density. The power density profiles are then used in the atomistic Momentum Scaling Model (MSM) coupled with the Molecular Dynamics (MD) method (MSM-MD) to predict the spatiotemporal evolution of WDP in vacuum. The spatial and

temporal distribution of density and temperature fields of expanding WDP is evaluated from the MSM-MD simulations. These modeling results provide insights into the underlining physics of the formation and spatiotemporal evolution of WDPs induced by cold X-rays.

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Introduction

When a nuclear blast occurs above the earth's atmosphere, most of the radiation produced from the detonation is in the form of X-rays because of the absence of atmosphere. The effects of X-rays from upper atmospheric nuclear detonations can potentially have severe and adverse impacts on satellite's solar panels and should be analyzed in order to evaluate the extent of the damage that can be caused. This thesis investigates the absorption of cold X-rays, which are low energy X-rays (~1-1.5 keV), by solar panel materials. Cold X-rays deposit the energy on the surface of materials. Therefore, they are harmful to solar panels of satellites in orbit because solar panels are extremely thin and complex pieces of equipment. If an excess amount of energy is deposited in the active semiconductor layer of a solar cell, this layer can melt, evaporate and expand as a dense plasma and short out nearby solar cells. If this occurs, the cost of repairing the orbital solar panels could be immense. This is why the effects of cold X-ray radiation from upper atmospheric nuclear detonations need to be examined in order to better understand the severity of repercussions that can occur.

The damage of electronic systems has been a concern for many industries where high levels of radiation are constantly present. In the fields of defense, nuclear power, and space exploration, radiation has been an important factor when considering the lifespan of machinery. Spacecrafts are designed to withstand a higher degree of radiation because there is no atmosphere to filter out the background space radiation. However, high altitude nuclear detonations can create a fireball that releases most of its energy through X-ray radiation, which can create photon fluences much higher than satellites are manufactured to withstand. These high-altitude detonations release 70 – 80 percent of their energy as X-rays which can damage electronic components on satellite solar cells [1]. In Conrad's technical report, *Collateral Damage to Satellites from an EMP Attack*, the

effects of radiation damage to electrical systems on satellites from previous tests of high altitude nuclear detonations is studied. Before the moratorium on atmospheric nuclear testing in 1963, multiple atmospheric nuclear tests were conducted. Some of these tests caused radiation belts in the atmosphere that directly led to electrical damage that shortened the lifespan of several satellites in orbit. One specific case of this was the STARFISH PRIME nuclear test, where the TRAAC and Transit 4B satellites stopped functioning due to decreased power output from their solar panels. This damage was caused by an artificial radiation belt induced by the nuclear test of STARFISH PRIME [2]. According to Fishell's study of this case, the satellite's solar cells had a large drop in power in the following month after the STARFISH PRIME test which resulted in their failure. This case provides an example of how the induced radiation from a nuclear detonation can cripple a satellites function and cause serious damage to the onboard electrical components.

With the advances in technology allowing for the development of more refined electronics, this has caused many of these electrical components to reduce in size and complexity. These micro-electronics are much more sensitive to radiation damage and current fluctuations. When radiation hits a material, it ionizes atoms causing electrons to be discharged. These electron vacancy's cause disruptions in the surface potential difference of materials which depending on the component can cause irregular current flow that can be extremely damaging [1]. This extreme sensitivity of electrical components will only increase with their complexity, meaning that radiation damage to these components will become a greater threat as technology advances.

The research done in the field of X-ray induced damage to solar cells has a very narrow breadth. Most of the information gathered has either been through the study of damage done on satellites after upper atmospheric nuclear tests in the late 50's and early 60's [1], or studies done in lab settings. While they do exist, the number of experiments is limited. One such study was

done in the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory (LLNL) [3]. In this study solar cell response to X-ray pulses was analyzed to better understand damages caused by nuclear weapons. A high intensity laser beam was shot at a target, ionizing it to create a source of X-rays [3]. The X-ray radiation was absorbed by a solar cell and current vs. voltage in the cell was measured. Surface defects were also analyzed to determine any damage done to the physical structure of the cell. The results of the study showed that the solar cell had no substantial degradation in performance, and the cover glass on the cell was still intact. There were, however, cracks that appeared in the cover glass. This response showed that the cover glass was effective at inhibiting damage into the solar cell because most of the energy deposited into the cell was extremely close to the surface on the cover glass [3]. The report concluded that more research needed to be invested into this topic to study the effects of radiation damage to solar cell arrays, because this study only examined single solar cell as the target.

What will be discussed in this thesis are the computational efforts made to better understand the effects of cold X-rays on solar panels of satellites in orbit. Most of the research has been completed using a computer code named GEANT4 [4], which is a simulation tool used for analyzing the interaction of radiation with materials. This code is used to predict the effects of cold X-rays on solar panels by examining the energy as well as the power density deposited by X-rays into materials of solar cells. The validation of the code used in this research was done through energy deposition profiles generated through experiments and computational methods [5]. The power density profiles are then used in a Molecular Dynamics (MD) simulation tool named LAMMPS [6], which can calculate how this power density deposited into the solar cells affects the material. Using these computational tools, a better understanding could be grasped on the damage that can be caused by cold X-rays on solar cells.

Chapter 1:

Physics of Radiation Interaction with Materials

1.1 X-ray and Electron Interactions with Atomic Electrons

Radiation damage is part of the field of nuclear physics. Radiation is considered a subatomic particle with high energy that causes ionization of material. To study the transport of radiation in materials, the physics of particle interactions needs to be examined. In this study X-rays are the main source of radiation, which use photons as the particle that is causing ionization. To better understand the effects of this radiation, the particle interactions from X-ray radiation that cause ionization will be analyzed.

When X-rays interact with an atomic electron there are a couple different effects that can result from their collision. For the purposes of this research only photoabsorption and Compton scattering are substantial because the results studied are concerned with energy deposited throughout the material at specific locations by cold X-rays. Interactions of photons with matter is based on the distance a photon can travel before a collision. The probability of this collision is a relation between the energy of the incoming photon and the atomic number Z of material, and is called the absorption cross section of the atom. The absorption cross section changes based on the energy of the incoming particle as well as the number density of atoms in a unit space. Based on this absorption cross section, a property called the mean free path can be calculated. The mean free path is in units of distance and describes how far a particle will travel inside of a material before it collides with an atom. Photoabsorption is the phenomena of a photon being absorbed into an atom resulting in the atom entering an excited state with an increased amount of energy. This increase in energy can then cause a secondary reaction which is the ejection of a photoelectron. Once a photon collides and is photoabsorbed that is the end of a photons path.

The probability of photoabsorption depends on the photoabsorption cross section of a material. This cross section involves the intensity of the incoming photon flux described as

$$I(x) = I_0 e^{-\Sigma x}$$

where $I(x)$ is the intensity of the photon flux at distance x inside the material, I_0 is the initial intensity of photons, Σ is the macroscopic cross section of interaction, and x is the distance into the material the photons have traveled. The macroscopic cross section is computed using the equation

$$\Sigma = N\sigma$$

where N is the atom number density of the material, and σ is the microscopic cross section of interaction based on the material and particle energy. These are both used to determine the collision density inside a material as

$$F = I\Sigma$$

where F is the collision density in units of (collisions/cm³·s). This gives the number of collisions that occur in a unit space per unit time [7].

Compton scattering is the other photon interaction process. It occurs when a photon collides with an atomic electron and bounces off, only transferring a portion of its kinetic energy to the electron. This will slow the photon down and change its trajectory. This phenomenon must be tracked because when a collision occurs a portion of the photon's energy is transferred to an electron, which is one of the main characteristics being studied. The relationship between the escape angles of an electron and photon is described as follows:

$$\cot \frac{\theta}{2} = 1 + \frac{h\nu}{mc^2} \tan \phi$$

where θ is the escape angle of a photon and goes from 0° to 180° , h is Planck's constant, ν is frequency of the photon, m is the mass of the electron, c is the speed of light, and ϕ is the escape angle of the electron which goes from 0° to 90° [8]. This along with the energy deposited by photoabsorption are what cause the energy deposition inside the material when exposed to X-ray radiation.

The last case examined for the relevant interactions was the production of secondary photons and electrons. The energy of the ejected electron is dependent on the energy of the incoming photon. The energy required to remove an electron from its orbital shell is related to the binding energy of the electron [8]. This means that the photon must have more energy than the binding energy of the electron to ionize it from its shell. This also means that the energy of the ejected electron is equivalent to the remaining energy of the incoming photon. Therefore, the energy of the electron is equal to the energy of the photon after removing the binding energy of the electron, which is seen in the equation below [8].

$$T = h\nu - B$$

where T is the kinetic energy of the emitted electron, h is Planck's constant, ν is the frequency of the photon, and B is the binding energy of the electron.

The electron response to radiation is an important reaction in the study of damage from radiation. When a highly energetic or charged particle collides with an electron it can result in a couple different reactions. When these particles interact a portion of energy is transferred from the particle in motion to the electron. This excited electron can either remain in the atom or be ejected from the orbital of the atom. If the electron is emitted, this loss of an electron is called ionization. The ionized atom now has a charge on it that can significantly affect the surrounding atoms.

Depending on which orbital the electron is emitted from an electron from a higher orbital can fall into the vacant spot in the lower orbital causing a release of energy in the form of a photon or Auger electron. The electrons that are emitted then can collide with other electrons. When the free electron loses energy, it emits photons with values of energy up to that of the energy loss from the electron. This effect of radiation produced from energy loss in electrons is called bremsstrahlung or braking radiation [9].

Another aspect of the physics that is important to understand is how cold X-rays interact with matter. Cold X-rays are X-rays with energies between 1 – 1.5 keV. This is an extremely low energy X-ray. As discussed earlier, the absorption cross section of an atom is directly related to the energy of the incoming particle. As the energy of the incoming photon decreases, the absorption cross section increases and the mean free path decreases. This means that there is a higher chance of the photon interacting with a particle after a shorter distance traveled while inside the material. For cold X-rays most of the energy deposited is within the surface layers of the material because of this. One of the main reasons for studying the effects of cold X-rays on the surface solar panels is because solar panels are extremely thin structures and most of the energy will be deposited on their surface, potentially causing material deformations.

1.2 Spectral Energy Distribution of Blackbody X-rays

The blackbody X-ray spectrum is used for determining initial energy of incident photons. It is the energy distribution that occurs from an upper atmospheric nuclear detonation. The incoming X-ray energies can be calculated using a spectral blackbody Planck function in terms of photon energy. This was derived from Planck function in terms of frequency which is written as

$$\frac{dN(\nu, T)}{d\nu} = \frac{2\pi\nu^2}{c^2} \frac{1}{\exp(h\nu/kT) - 1} \left[\frac{1}{\text{cm}^2 \cdot \text{s} \cdot \text{Hz}} \right]$$

where ν is the photon frequency, $h = 4.1356677 \times 10^{-18} \text{ keV} \cdot \text{s}$ is Planck's constant, $c = 2.99792458 \times 10^{10} \text{ cm/s}$ is speed of light, $k = 1.380649 \times 10^{-23} \text{ J/K}$ is Boltzmann's constant, T is temperature, and $kT [\text{keV}]$ is thermal energy. This spectral photon flux can be written in terms of photon energy $\varepsilon = h\nu$ as

$$\frac{dN(\varepsilon, T)}{d\varepsilon} = \frac{2\pi\varepsilon^2}{c^2 h^3} \frac{1}{\exp(\varepsilon/kT) - 1} \left[\frac{1}{\text{cm}^2 \cdot \text{s} \cdot \text{keV}} \right]$$

The photon flux, i.e. number of photons emitted per second per unit surface area of a blackbody, can be obtained by numerical integration taken over the corresponding spectral energy intervals

$$N(\Delta\varepsilon_i, T) = \frac{2\pi}{c^2 h^3} \int_{\varepsilon_i}^{\varepsilon_{i+1}} \frac{\varepsilon^2}{\exp(\varepsilon/kT) - 1} d\varepsilon \left[\frac{1}{\text{cm}^2 \cdot \text{s}} \right]$$

The numerical integration was performed using an accurate method of Gaussian quadratures. This gave a relationship between photon flux and photon energy. These energy and flux arrays that were mapped to each other were then used to create a probability density function to give an accurate estimation of the flux and energy values for each incoming photon. If the thermal energy is 1 keV the temperature is approximately $12 \times 10^6 \text{ K}$. The total summed flux for this energy is approximately $2.4 \times 10^{32} \text{ ph}/(\text{cm}^2 \cdot \text{s})$. This value can be calculated numerically using the following equation.

$$F_{ph} = \frac{4\pi\zeta(3)}{c^2h^3}k^3T^3 \approx 2.38 \times 10^{32} \left[\frac{ph}{cm^2 \cdot s} \right]$$

where $\zeta(3) \approx 1.2$ is known as Apéry's constant. This lets us compare the calculated flux to a numerically found flux value to validate this method for defining flux values.

Chapter 2:

Computational Models

2.1 Monte-Carlo Method

The Monte-Carlo (MC) method is a computer-based model of simulation using random sampling to produce accurate results in probability based problems. Particle interactions are simulated using this method because they work on a probabilistic model that changes based on the parameters of the problem being examined. The different physical properties present in which particles interact change the probabilities of interaction. Factors such as initial energy of the incoming particle, mass density of the material they interact with, as well as distance to the target all impact the probability of interaction. This is why a MC simulation is used in this research, to generate accurate results for a problem that can only be examined theoretically.

The modeling of X-ray interactions with materials is an extremely computer resource intensive process. Each photon produced by the source has to be followed, and the path that the particle takes is estimated based on a probabilistic model, the Monte-Carlo simulation. This simulation uses the characteristics of the incoming photon as well as the material it is going to interact with to determine how the photon will behave. In the simulation conducted for this research the different types of interactions considered were photoabsorption, Compton scattering, and the production of secondary photons and electrons.

When using the Monte-Carlo method of simulating particle interaction, a couple parameters need to be established. The first being the source of photons. When considering the source, the initial energy of the photon must first be set. The properties of the target must also be

set. These initial parameters are needed in order to properly run a MC simulation. However, this method is extremely time and resource intensive. This is because modeling these interactions is based on probability. If only one hundred particles from the source X-ray are followed, the probability distribution of how these particles interacted would almost certainly be wrong and would not produce a smooth trend. In order to increase the accuracy of a Monte-Carlo simulation an extremely large number of particles should be followed. The variance of this simulation can be described as

$$\sigma^2 = \frac{1}{N}$$

where σ^2 is the variance of the simulation, and N is the number of runs [10]. Variance describes the deviation from the mean value in probability theory. This relationship is derived from the Gaussian distribution applied to statistical analysis, which is used in approximating a distribution drawn from many outcomes and samples [10]. It shows that as the number of samples increases, the deviation from the mean also decreases.

2.2 Set up of Geometry

In this study, the effect of cold X-rays on a solar cell assembly was considered. The way in which the geometry of the solar cell was established is based on information provided by the US Naval Research Laboratory. The schematics of the solar cells is shown in **Figure. 1**, and the thickness, composition and mass density of each layer is reported in **Table 1**.

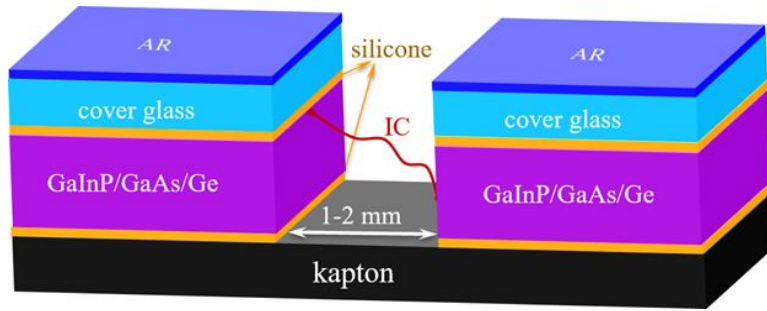


Figure 1: Solar Cell Configuration

Layer	Material	Thickness (μm)	Composition	Mass Density (g/cm^3)
1	Anti-Reflective (AR) Coating	.12	MgF_2	3.148
2	CMX Cover Glass	100	SiO_2(63.6%) B_2O_3(10.4%) ZnO(4.5%) BaO(2.7%) K_2O(7.7%) Al_2O_3(4.7%) CeO_2(4.6%) U_3O_8(1.8%)	2.6
3	Silicone Adhesive DC 93-500	12	$\text{CH}_3[\text{Si}(\text{CH}_3)_2\text{O}]_n\text{Si}(\text{CH}_3)_3$ *n is number of repeating monomer units	.965
4	Active Semiconductor	0.8 (GaInP) 3.6 (GaAs) 300 (Ge)	*Layer is composed of 3 subsections of GaInP, GaAs, and Ge	4.475 (GaInP) 5.32 (GaAs) 5.3234(Ge)

Table 1: Thickness, Composition and Mass Density of Solar Cell Layers

Using this information, a virtual box comprised of slabs representing each layer was constructed. The Kapton substrate was not included into the simulations of the solar cell because it is a substrate and any energy that penetrated this layer was considered not essential for the purposes of this research.

The other case that was studied corresponds to different angles of incident X-ray radiation onto the unshielded Germanium active semiconductor layer. This was done in order to examine how incident radiation on the unprotected side of the semiconductor would damage the component. The different angles are used to mimic the satellite being in different orientations with respect to the source of the nuclear detonation. This is the case that will be run through LAMMPS in order to study how the material reacts to the power density distribution imposed by the cold X-ray radiation. This will show whether the material will ablate and potentially interfere with adjacent solar cells. For this case a single layer of Germanium with thickness 5mm was exposed to direct 1 keV X-ray radiation at 10, 45, and 80 degree angles of incidents. The setup of this case can be seen in **Figure 2**.

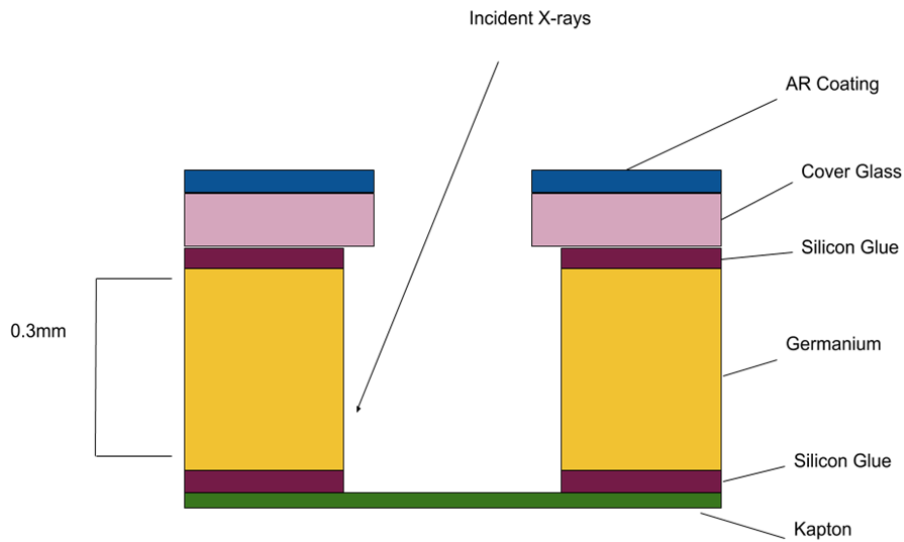


Figure 2: Schematic of incident X-rays interacting with Germanium slab

2.3 MC Simulation using GEANT4

The Linux based computational physics software called GEANT4 is used to perform the MC simulation of X-ray transport in solar cell materials. GEANT4 is a computer program written and compiled in the C++ coding language. The GEANT4 software package includes the libraries containing the physical properties of many different materials as well as the cross sections and interaction processes of photons and electrons with atoms. The MC simulation of the transport of X-rays and secondary particles in materials is implemented into the GEANT4 software for conducting this research. The computer code development has involved the implementation of the spectral energy of blackbody X-rays, the multi-slab system to mimic a solar cell, different angles of incident X-rays into the active semiconductor layer of the cell, as well as the way in which data is collected as output from this computer code.

The first addition made onto the basic version of GEANT4 was the creation of a multi-slab system. Meaning that the program was changed from X-rays being shot at a box of one material, to a box of multiple layered slabs. These slabs were coded to be comprised of the same material and possessing the same material properties as the different components of the solar cell show in **Figure 1** and **Table 1**. The slabs were then arranged and sized to match that of a single solar cell. This meant that the X-rays shot at the target material were being shot incident to a solar cell replica, and energy from these X-rays could be output based on depth of penetration across the system.

The next piece of code that was implemented was the method of collecting data. Collection of data had to be constructed for this research because the output of this simulation needed to be in an easy to use format so it could be displayed, and later used in the Molecular Dynamics software LAMMPS. The output of this simulation was two different energy distributions. The first

distribution was the averaged energy deposited at each point across the slabs. Energy deposition was calculated based on the total energy deposited at each point across the depth of the slab, and then divided by the total number of particles that were followed during the simulation. This gave an energy deposition profile across the array of slabs that comprised the solar cell and can be seen in **Figure 4** in the results section of this paper. The other output for this simulation was the power density distribution of the X-rays across the solar cell array. Power Density used the spectral distribution of blackbody X-rays to incorporate a time variable into the output. Rather than energy deposited at each point, the power density at each point across the depth of the solar cell array was calculated and output.

This method of data collecting was also used in the single slab of Germanium case as well. The changes made to the code for this case were the angle of incidents as well as reverting the simulation to a single slab system. Different angles of incidents were implemented by using direction cosines to input the angle of the incoming particles. The energy deposition, power density distribution, as well as the information produced from the Molecular Dynamics software LAMMPS being fed into a visualization software called PyMol will be discussed in the results section.

The last piece of code that was implemented was the spectral distribution of blackbody X-rays. The math behind this code was explained earlier in this thesis in section *1.2 Spectral energy distribution of blackbody X-rays*. This code allowed for the flux of each particle based on initial energy to be calculated and used for the power density distribution output. The flux of the particles involves a time variable, which then allowed for the calculation of the power density at each point along the solar cell array.

2.4 Molecular Dynamics Simulation

Molecular Dynamics (MD) numerically models the motion of discrete atoms. There are many different applications of MD modeling, and here it will be used to analyze the response of the active Germanium semiconductor in the solar cell to different angles of incident X-rays. MD modeling was first used to simulate complex fluid interactions and was later used to model proteins [11]. Since then it has been expanding to fields of study in material science with the improvement in computational power, which allows for more atoms in simulations, and longer time intervals in runs. The MD modeling is used to improve understanding of how the physical material in solar cells responds to deposited energy from X-rays.

The MD code being used is LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) which is a program developed for materials modeling as well as many other applications such as atomic, polymeric, biological, solid-state, etc. [5] The Momentum Scaling Model (MSM) was coupled with the MD method (MSM-MD) and implemented in LAMMPS to predict the ablation of materials by femtosecond laser pulses [12]. This MSM-MD approach was adapted and used to model the interaction of X-rays with solar cell materials. The input for LAMMPS is the power density distributions derived from GEANT4, which is used to model how the atoms in the Germanium semiconductor would respond and move after being exposed to that distribution of energy. The way the program is set up is by establishing the box that represents the environment for the MD case. This is done by establishing the lattice structure of the material, which is diamond for Germanium, as well as the lattice period which is the length in angstroms between each repeated lattice cell in the material. Then the number of times that this lattice is repeated in the X, Y, and Z direction of the box is declared. The energy profile from GEANT4 is then input into LAMMPS and the atoms inside the box are processed in the MD numerical

simulation to show how the atoms would move according to the material parameters and energy profile. This simulation will then output time moments of the material in the form of coordinates of the different atoms within the material that can be visualized with the help of PyMol. These results show the severity of material blow off from the different situations established in GEANT4.

Chapter 3:

Results

3.1 Results from GEANT4

Multiple test cases were run through the GEANT4 simulation of incident X-ray on the solar cells. The three cases were differentiated by the initial thermal energy of the photons which were 0.1, 1, and 10 keV. Each case had a probability density function (PDF) created based off the spectral Planck function for photon energies. The distribution of flux for each case as well as their PDF's are shown below.

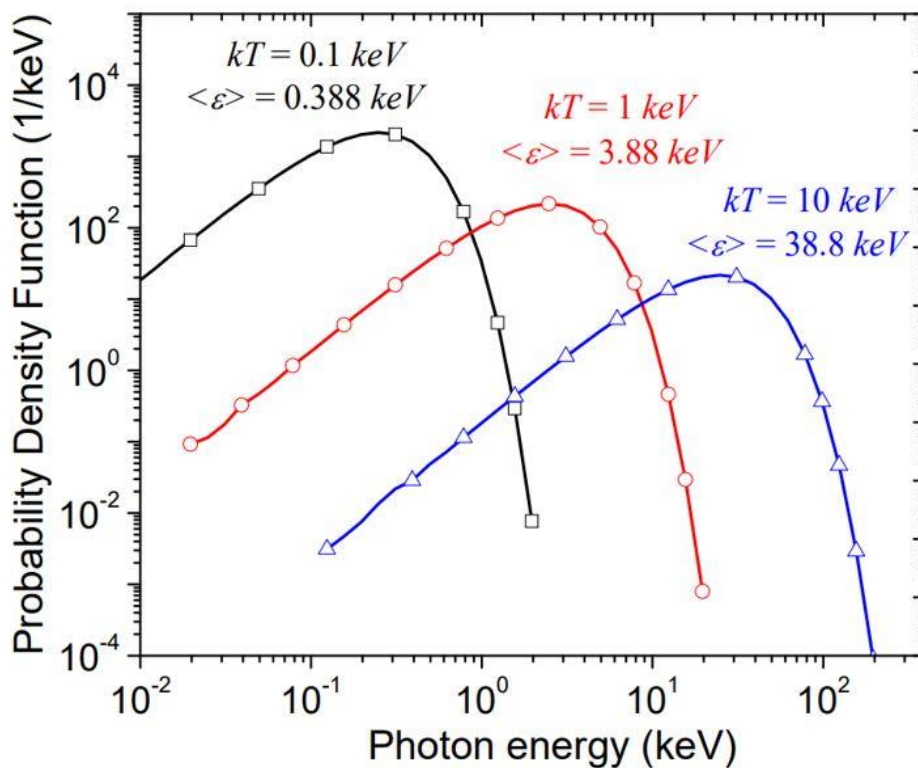


Figure 3a: Probability Density Function for the three thermal energy cases

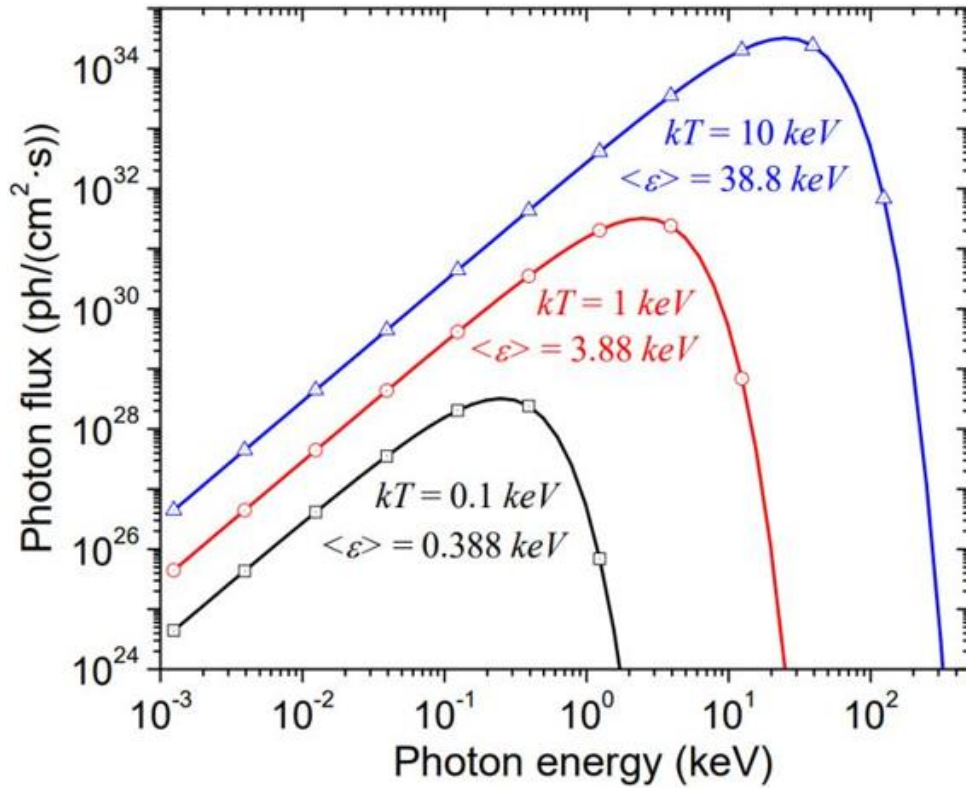


Figure 3b: Distribution of photon flux based on Planck's function

These plots show us that lower energy photons also have a lower flux from **Figure 3b**, but the probability of the incident photon having energy close to the mean value is also higher.

Using the PDF of photon flux the different simulations could then be conducted. The first runs were energy deposition. The results from the energy deposition case are shown below in **Figure 4**.

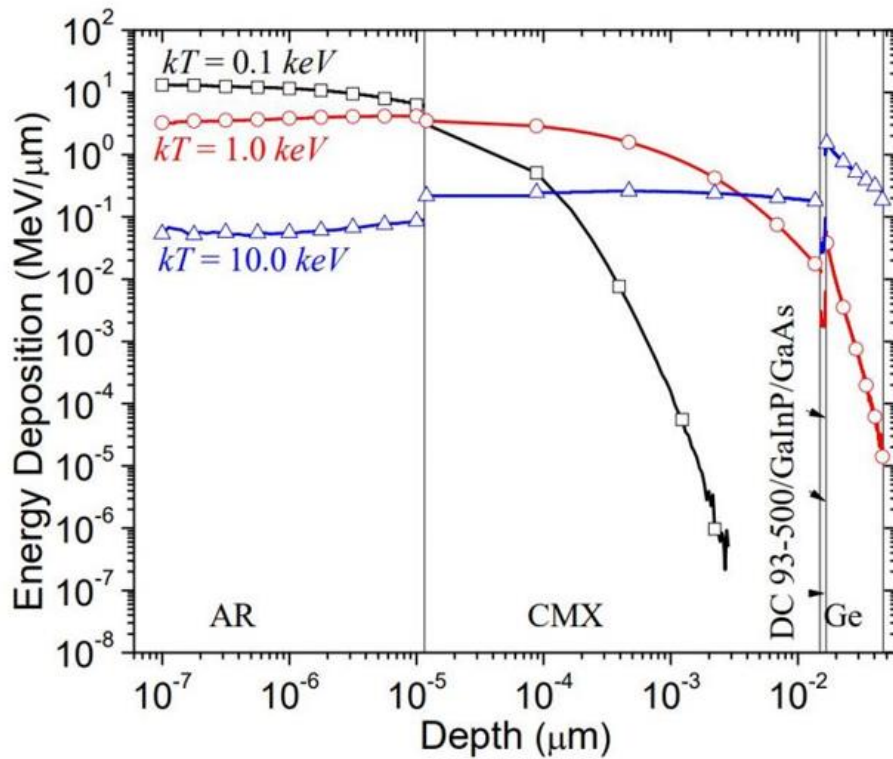


Figure 4: Energy Deposition profile across solar cell

The graph of energy deposition shows the energy deposited vs. the depth into the solar cell. The vertical lines represent the boundaries between the slabs. At these boundaries there are small discontinuities in the energy deposited for each case. This is a result of the different material properties changing the probability of interaction in the material. As the photons pass through the boundary of two layers, the probability of interaction changes as well, resulting in small jumps in deposited energy. From these graphs it is also clear that the lower energy X-rays deposit more total energy towards the surface of the material but also have less penetration into the material. Comparing the 0.1 keV and 10 keV cases, the 0.1 keV X-rays does not penetrate past the cover glass layer (CMX), while the 10 keV X-rays appears to have deposited a large amount of energy into the active semiconductor portion of the cell (Ge) and even had photons penetrate past this

layer. The 1 keV X-rays, which are the X-rays that have energy closest to that of the cold X-rays produced from a nuclear detonation also show energy deposited into the active solar cell component. This means that some of the energy did accumulate in this region and could potentially cause damage to the cell.

The next portion of data that was collected was the power density distribution across the solar cell. The same three cases were run to collect this data and were converted to incorporate the flux of the incoming particles into the data collection process. The figure below shows the results from this run.

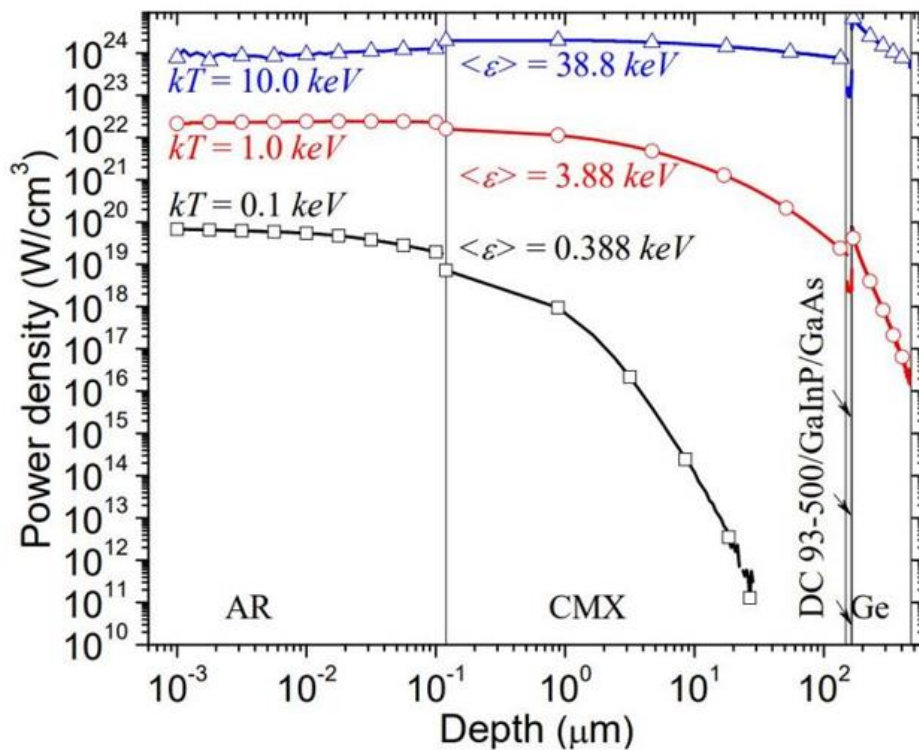


Figure 5: Power density distribution across solar cell

This graph shows the power density of the three thermal energy X-ray simulations across the solar cell. From this a different interpretation of the X-ray penetration compared to the energy deposition

profiles can be observed. Here the power density present in the surface anti-reflective (AR) layer of the solar cell is higher for the 10 keV X-rays, where in the energy deposition profile the 0.1 keV X-rays had the most energy deposited here. This can be explained with the graph of photon flux's in **Figure 3b**. Looking at this distribution, the flux of X-rays with blackbody temperature of 0.1 keV at its peak is six orders of magnitude lower than the peak of the 10 keV X-rays. This means that there is a much greater number of photons interacting with the material in the 10 keV case every second. Because of this the power absorbed by the solar cell is much higher than the 0.1 keV case, even though the 0.1 keV case deposits more total energy over the run. This graph also shows that there is a high power density in the active solar cell component for the 1 keV case. These results give more evidence that the X-rays from an upper atmospheric nuclear explosion could potentially harm a solar cell array attached to a satellite.

The other case examined through GEANT4 was the effect of different angle of incidence into the active solar cell component comprised of Germanium. This was done to show how at different satellite orientations to the nuclear explosion, X-rays could directly interact with the Germanium layer of the solar cell through the unshielded gaps between the cells. Three different cases were run to better understand this scenario: 10, 45, and 80 degrees from the surface. The results in the form of a power density distribution graph are shown below in **Figure 6**.

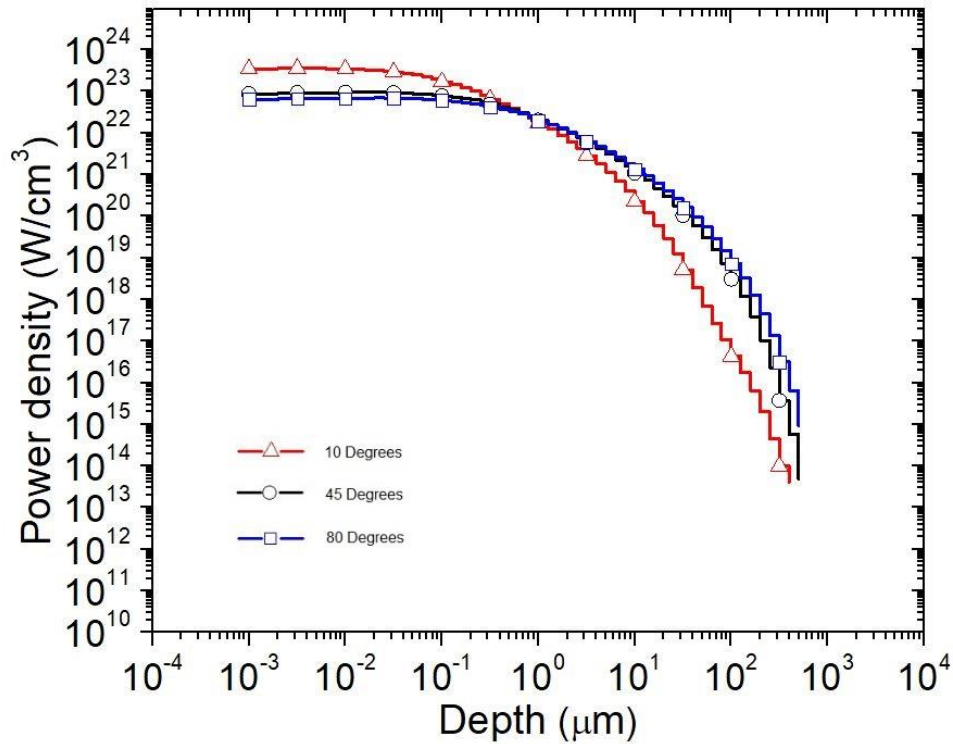


Figure 6: Power density distribution of different angles of incidence into Germanium layer

Figure 6 shows the power density profiles of 1 keV X-rays incident at the three different angles into the unshielded Germanium slab. As expected, the shallow angle of 10 degrees from the surface of the material has the highest power density closest to the surface of the material, but also penetrates the least. Conversely, the 80-degree X-rays have the deepest penetration but lowest power density close to the surface. This is due to the geometry of the X-rays colliding with the material. For the 10-degree X-rays, the X-rays are almost parallel to the surface of the material, causing most of the X-rays to interact somewhere close to the surface. This also caused the rapid drop off in energy deeper into the Germanium slab because all the photons were interacting close to the surface, and therefore, did not have enough energy to penetrate deeper into the slab. The 80-degree case is the opposite of this. Because the 80-degree case was close to a directly straight on

interaction, the photons could travel farther into the material before interacting, resulting in the trend shown in **Figure 6**. Another interesting result from this graph was the 45-degree case. It is almost identical to the 80-degree case with just a little more power density close to the surface and a slightly shallower penetration. It appears that as the angle increases the change between the cases decreases.

3.2 Results from LAMMPS

The MD simulations in LAMMPS use the power density profiles created in GEANT4 as inputs for the MD simulation. Using these power density distributions, a visual representation can be created of the material response to the X-ray interactions. LAMMPS' MD simulation output is in the form of XYZ coordinate file, containing the position of particles in the Germanium slab at different moments. The time moments that best show the material reaction are shown below in the following figures which were output using the visualization software PyMol.

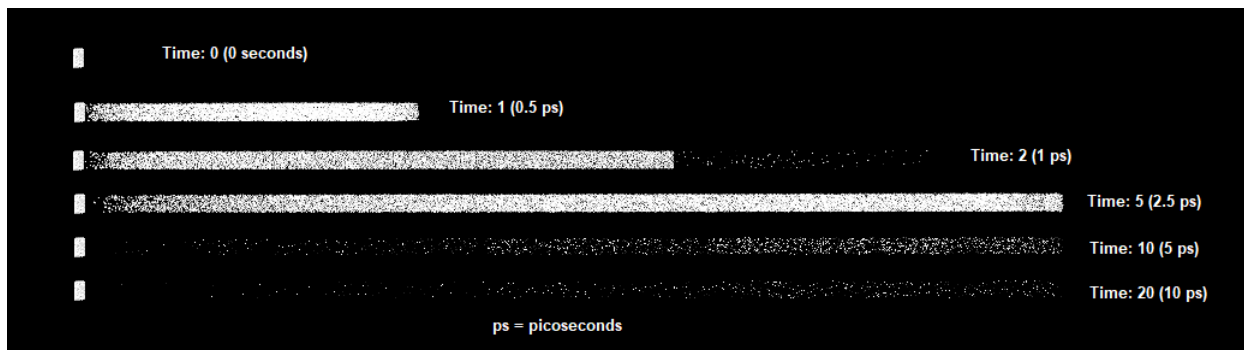


Figure 7: MD results from 10 degree case

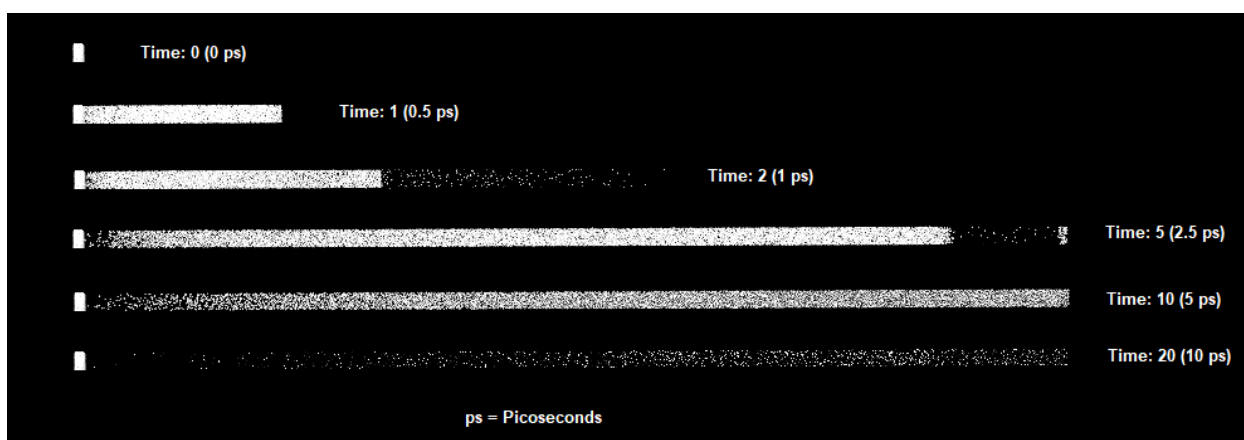


Figure 8: MD results from 45 degree case

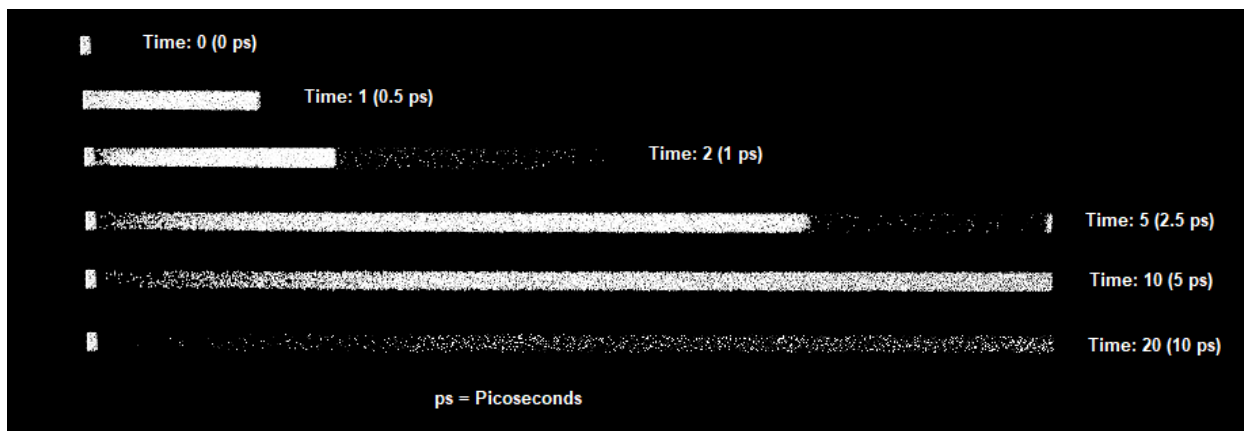


Figure 8: MD results from 80 degree case

The figures shown contain a couple time moments of the simulations that demonstrate the differences as well as similarities between the different cases. Initial time moment of 0 picoseconds (ps), as well as 0.5 ps, 1 ps, 2.5 ps, 5 ps, and 10 ps are shown in each case for the sake of comparison. These times represent the iterations of the MD simulation which were output periodically. Each time snapshot occurred after 500 iterations of this simulation, where each iteration is equal to 0.001 picoseconds (ps). The small white rectangle on the left side of each time moment is the surface of the Germanium slab. LAMMPS stopped the simulation at the 20th time moment or 10 picoseconds, which is shown in each case.

Looking at the cases for different angles of incidence the results from the MD simulation follow what would be expected from the power density profiles produced in GEANT4. The case of 10 degrees had the highest power density at the surface of the material, which caused a larger and faster blow-off of material from the Germanium slab. Time 0.5 ps from the 10-degree case has particles ejected at a further distance than the other two cases. This becomes more obvious at time 1 ps and 2.5 ps where their position across the computational domain is much greater in the 10-degree cases compared to the 45-degree and 80-degree cases. At time 2.5 ps the 10-degree case has material reaching and most likely extending past the computational domain of LAMMPS while the other two cases have not reached the end of the domain. The latter time 5 ps the ejected particles are already starting to leave the domain all together for the 10-degree case, but for the others there is still much of the ejected matter present, and it does not appear to leave the domain until time 10 ps.

These results from LAMMPS validate the assumptions made from the power density profiles in GEANT4. Because of the high power density more damage was expected to occur from the 10-degree case, while the 45 and 80-degree cases were close to identical with only slight

variation and less severe material ejection. LAMMPS has proven to be a useful tool to help validate the assumptions made based off the power density profiles generated in GEANT4.

Conclusions

The results on the energy deposition and power density derived from GEANT4 as well as the MD simulations using LAMMPS provide the understanding of the material response to cold X-rays produced by upper atmospheric nuclear detonations. The results of power density from the simulated solar cell being irradiated with different temperature X-rays shows that the effects of cold X-rays can potentially be damaging to the active layer of a solar cell. The case of X-rays with blackbody temperature of 1 keV is important here because it shows that energy produced from a nuclear detonation can penetrate this active layer and potentially cause blow off of material and the formation of warm dense plasma. The difference between the energy deposition and power density profiles, where blackbody 10 keV X-rays have the least energy deposition and most power density close to the surface, is due to the photon flux. The 10 keV X-rays has a flux that is six order of magnitude greater than that of the 0.1 keV X-rays. This is why even though the 10 keV X-rays had lower energy deposited in the front layer and also higher power density. The number of X-rays depositing energy per unit time was much greater because of the number of photons being shot into the cell per unit time.

The simulation of different angles of X-rays incident directly onto the active layer of the solar cell show how the orientation of the satellite can affect the power density distribution into the semiconductor component of the solar cell. At very shallow angles most of the power density is absorbed very close to the surface, meaning that the surface material is much more likely to blow-off and potentially disable the solar cell. While a large power density still deposited at steeper incident angles in the surface and can still damage the cell, they cause less damage compared to a shallow angle where all the power is deposited at the surface of the material. The drop-off of power

density deeper into the cell is also a result of the angle of incidence. This is another result that shows how the shallow angles cause all the X-ray's power to be distributed close to the surface, creating a larger change of material blow off.

Future considerations for this research would be using the power density distributions from GEANT4 for the full solar cell and simulate the MD response in LAMMPS to study the material –blow-off for the entire solar cell. Using the power density profile from GEANT4 for the whole solar cell in an MD simulation would provide an idea of how the solar cell would respond, and if any blow-off would appear. Then using the MD results from both cases, the electrical and thermal properties of these material ejections could be studied to discover if they would damage adjacent solar cells. Using this information, new methods of shielding solar cells could be analyzed and implemented to protect solar cells on satellites from cold X-rays produced by upper atmospheric nuclear detonations.

Author's presentations: conferences

1. Fogleman M. and G. Miloshevsky. *Power Density Distributions Produced by Cold X-rays in Multi-Layer Slab Targets*. 2019 DTRA Radiation Effects Technical Review, Ballston (Arlington), VA, June 25, 2019.
2. Fogleman M., C. Wenzel, and G. Miloshevsky. *Dynamics and Properties of High-Density Surface Plasmas Induced by Cold X-rays*. The 10-th International Workshop on Warm Dense Matter (WDM 2019), Travemünde, Germany, May 5 - 9, 2019.
3. Fogleman M. and G. Miloshevsky. *Energy Deposition Distributions Produced by Cold X-rays in Multi-Layer Slab Targets*. Abstracts of the 22nd Annual Graduate Research Symposium, Virginia Commonwealth University, Richmond, VA, April 23, 2019, P13.

References

- [1] Conrad, et al. "Collateral Damage to Satellites from an EMP Attack." *Apps.dtic.mil*, Defense Threat Reduction Agency, Aug. 2010, <https://apps.dtic.mil/docs/citations/ADA531197>.
- [2] Fischell, Robert E., et al. "SOLAR CELL PERFORMANCE IN THE ARTIFICIAL RADIATION BELT." *AIAA Journal*, Aerospace Research Central, 17 May 2012, <https://arc.aiaa.org/doi/full/10.2514/3.1518>.
- [3] Jenkins, Phillip P., et al. "Nuclear Weapons Effects Testing of Solar Cells Using the National Ignition Facility (NIF)." *2010 35th IEEE Photovoltaic Specialists Conference*, 2010, doi:10.1109/pvsc.2010.5614573.
- [4] Agostinelli, et al. "Geant4-a Simulation Toolkit." *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, North-Holland, 11 June 2003.
- [5] Miloshevsky, Gennady, and Caffrey, J. A. *Electron Deposition and Charging Analysis for the Europa Lander Deorbit Stage*. NASA Technical Report, (2019), in press.
- [6] Plimpton, Steve. Fast Parallel Algorithms for Short-Range Molecular Dynamics, *J Comp Phys*, 117, 1-19 (1995), <https://lammps.sandia.gov/>.
- Knief, Ronald Allen. *Nuclear Engineering: Theory and Technology of Commercial Nuclear Power*. American Nuclear Society, 2008.
- [7] Lamarsh, John R., and Anthony John Baratta. *Introduction to Nuclear Engineering*. Prentice Hall, 2009.
- [8] Nikjoo, Hooshang, et al. *Interaction of Radiation with Matter*. Taylor & Francis, 2012.

- [9] Turner, James Edward. *Atoms, Radiation, and Radiation Protection*. Wiley-VCH Verlag GmbH & Co. KGaA, 2010.
- [10] Landau, David P., and K. Binder. *A Guide to Monte Carlo Simulations in Statistical Physics*. Cambridge University Press, 2015.
- [11] Deuffhard, Peter. *Computational Molecular Dynamics: Challenges, Methods, Ideas: Proceedings of the 2nd International Symposium on Algorithms for Macromolecular Modelling, Berlin, May 21-24, 19997*. Springer, 1999.
- [12] Miloshevsky, Alexander, et al. "Generation of Nanoclusters by Ultrafast Laser Ablation of Al: Molecular Dynamics Study." *Physical Review Materials*, vol. 1, no. 6, 2017, doi:10.1103/physrevmaterials.1.063602.