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SPATIO-TEMPORAL EVOLUTION OF WARM DENSE PLASMAS: MOLECULAR DYNAMICS MODELING

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Abstract

The exo-atmospheric detonation of nuclear device would be of great impact on the material integrity of orbiting satellites. The spectral energy distribution of high intensity X-ray flux, ~10^{28}-10^{35} photons/(cm^2·s), originating from a nuclear blast is described by the Planck's blackbody function with the temperature from 0.1 keV to 10 keV. Particular damage would occur to the multi-layered, solar cell panels of satellites. However, the X-ray flux incident upon the solar panels is inversely proportional to the square of the distance from a point where a weapon was detonated. For example, the X-ray flux is reduced by a factor of 10^{-10} at the distance of 100 km. Even accounting for this geometric factor, the enormous power density, ~0.1 - 10^4 GW/cm^3, absorbed within a few microns of a Ge slab of solar cells produces the extreme pressures and temperatures. The X-ray induced blow-off and Warm Dense Plasma (WDP) formation on the surface of materials, particularly in a gap between the unshielded Ge elements is initiated. In this work, the profiles of deposited energy and power density produced by cold X-rays (~ 1 keV) in the multi-layered materials are calculated using the Monte Carlo method within the *Geant4* software toolkit. The power density is used as an input for the Molecular Dynamics (MD) modeling of WDP formation and expansion into vacuum. The MD computational model is implemented within the *LAMMPS* software toolkit. The spatio-temporal evolution of WDP as well as its temperature, stress, and mass density distribution are investigated for different X-ray irradiation conditions.

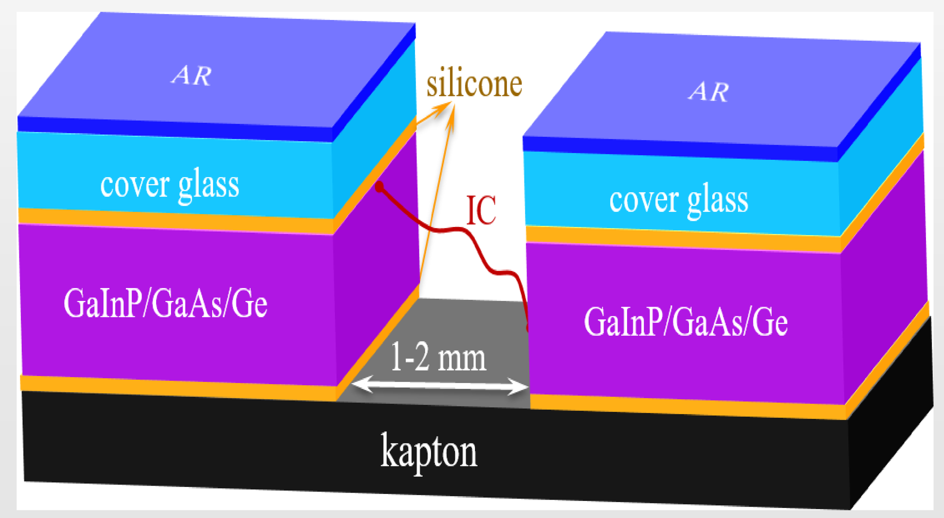
Background and Motivation

The primary goal of this project is to gain a better understanding of how a high altitude nuclear explosion would affect satellites. Of specific interest is the damage induced by radiation on the solar panels which power these satellites. By understanding how satellite solar arrays are affected by X-rays we may be better prepared in the case of a thermonuclear detonation beyond the Earth's atmosphere.

- **Goal of research:** gain a better understanding of the effects by cold X-rays with blackbody energy spectrum on the surface of solar cell materials
  - Analyze development of WDP
  - Simulate material ejection using MD techniques

Computational Model

- **GEANT4**: software toolkit developed by CERN for the simulation of the transport of particles through matter
- **LAMMPS**: Molecular Dynamics (MD) software used to simulate spatio-temporal evolution of target material after X-ray flux exposure



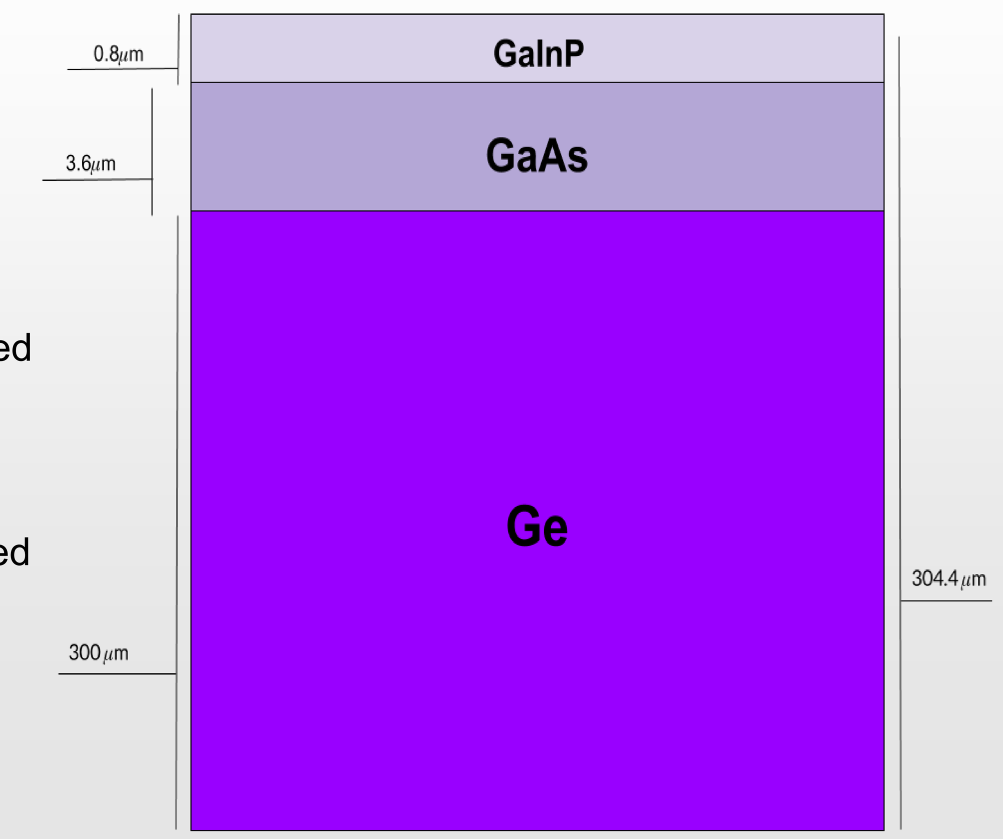
Multi-Slab Target Geometry

- Target comprised of a multi-slab system: developed in order to simulate X-ray interactions with satellite solar cells; the primary target however was a slab of Germanium
- Primary generated X-rays: sampled from blackbody spectrums with temperatures of 0.1, 1, and 10.0 keV
- Molecular Dynamics Simulation: The MD simulation performed within the LAMMPS code library utilized GEANT4 power density profiles, so as to generate WDP density and temperature maps

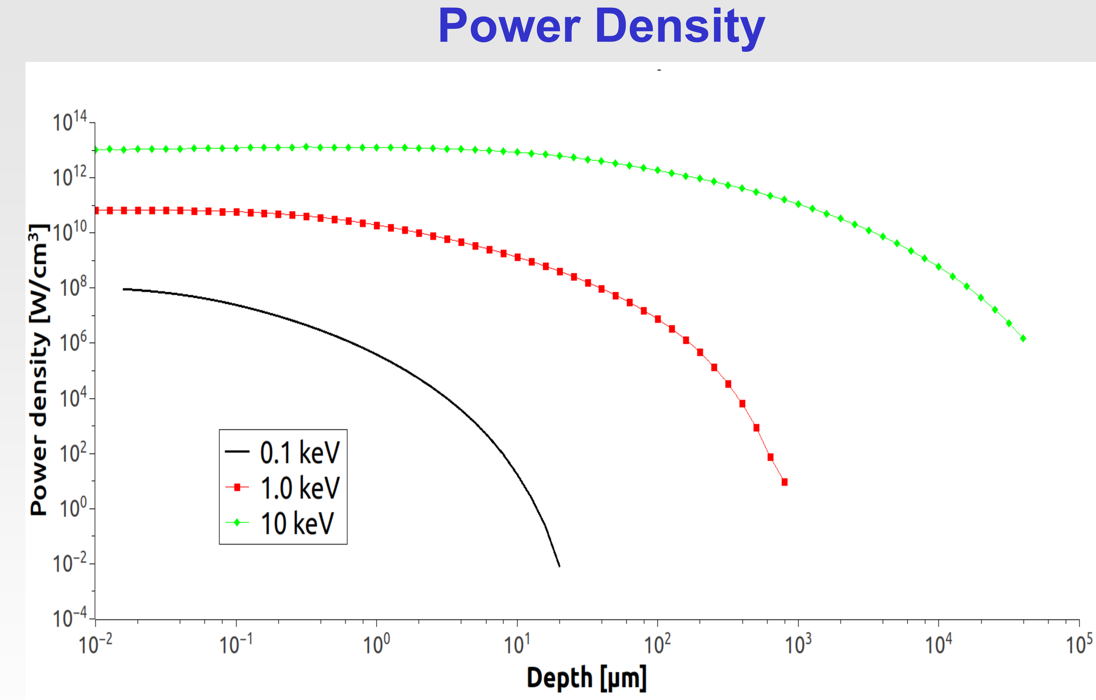
Power Density Profiles of 0.1, 1.0, and 10.0 keV Blackbody X-ray Fluxes onto the Germanium Active Component

Target Geometry

- Active semiconductor solar component consists of 3 sub layers.
- Majority of the active semiconductor is Germanium (98%)
- Simulations utilize a target geometry comprised of 100% Ge.
- All 3 power density profiles have a similar, nonlinear curvature.
- Geometric attenuation factor of 1e-10 is utilized in order to account for an assumed target / explosion separation of 100 km.

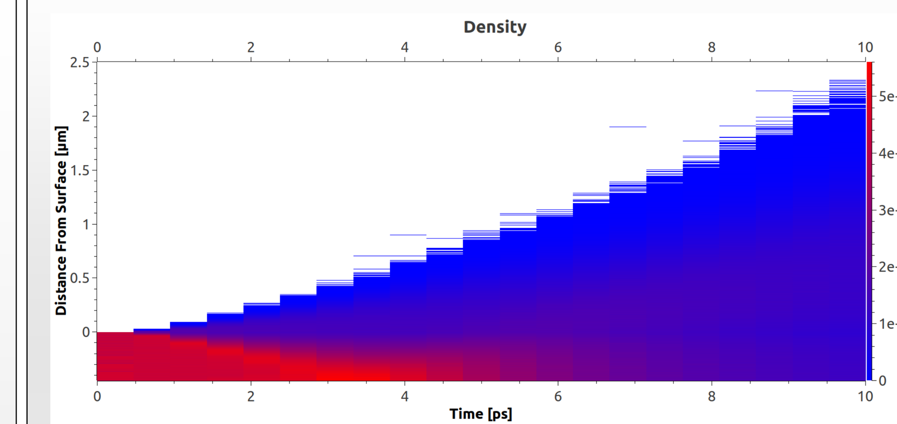


Power Density



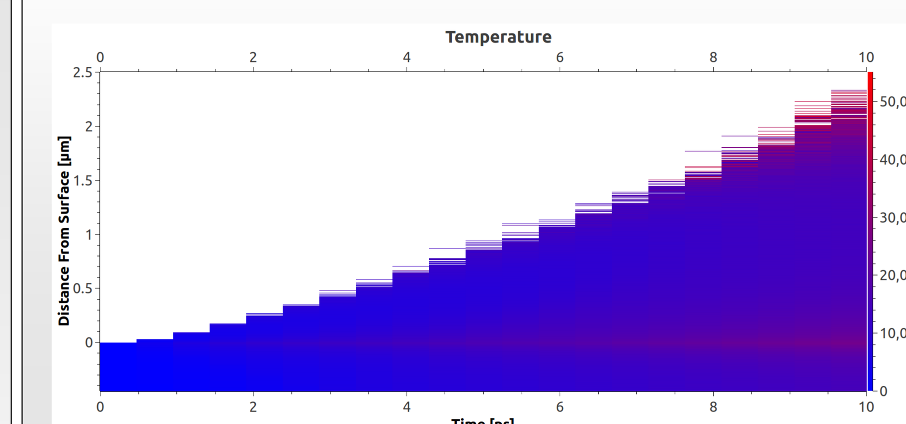
- The 0.1 keV blackbody X-rays can deposit a dose to around ~ 20 micrometers deep, the 10.0 keV blackbody X-rays can deposit a dose to a depth ~5 to 7 orders of magnitude greater.
- Power density may be evaluated by considering the flux of each particle as obtained via the simulated 0.1, 1.0, or 10.0 keV temperature blackbody spectrum.
- The power densities (Dose Rates) characteristic of these oncoming cold X-rays will determine the manner in which the solar instrumentation is damaged

Density Map, 0.1 keV Blackbody



- WDP: generated in regions of density between 2e+22 and 3e+22 atom/cm^3
- Target Material Ejection: ablation of target forces material to be ejected up to ~2.3 micrometers during 10ps after initial exposure.

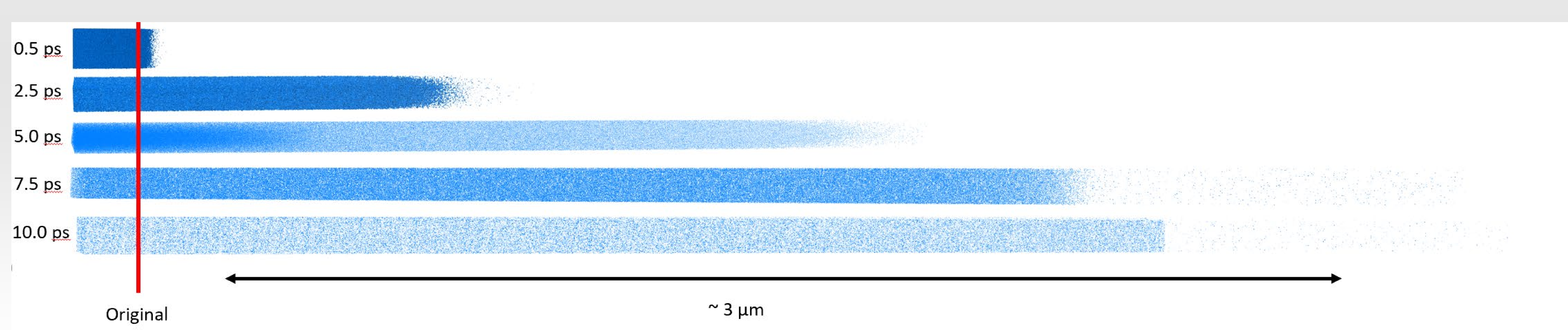
Temperature Map, 0.1 keV Blackbody



- High Temperature Front: Low density, high temperature Plasma is observed to be ejected furthest from the target surface after ~10 ps of exposure
- WDP: has temperatures ranging from ~1 to ~ 100 eV

Molecular Dynamics Parameters and Results

- The Germanium target geometry has a diamond structure with a lattice parameter of 5.658 Angstroms.
- Target dimensions 40 x 40 x 800 lattice parameters or 226.3 x 226.3 x 4526.4 Angstroms.
- Z-Bottom of MD box utilizes reflective boundary, X and Y boundaries are periodic.
- Material ejected ~ 3 µm
- Lower density, higher temperature plasma can be observed far beyond the original surface after 5 ps.
- WDP visible beneath and beyond original surface in 10ps model.



Conclusions

- 0.1 keV X-rays reach a depth of ~20 micrometers while the 1.0 keV X-rays reach a depth on the order of 1mm. The 10.0 keV X-rays achieve a depth of ~ 50mm.
- The 10 ps evolution allows sufficient time for the generation of WDP beneath the front of initially ejected material.

Future Work

- Analysis of layer interfaces both within and without the active solar cell component
- Study the formation and time-space evolution of internal shockwave generated by ablation of material and formation of WDP.

Acknowledgment

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