Title: ION TRANSPORT CALCULATIONS USING MCNP

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Ion Transport Calculations using MCNP

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The MCNP\(^1\) Monte Carlo code (version 4B) has been adapted to perform multi-dimensional ion transport calculations in amorphous media for microelectronics materials applications. In this application, focused ion beams are used to implant donor ions through a mask into an underlying semiconductor substrate, achieving tailored implantation profiles as a function of penetration depth with a minimum of radial spread past the mask edge. However, as the device feature size shrinks below submicron scale, this radial migration of ions becomes important. Our goal is to simulate ion implantation in materials containing two and three dimensional heterogeneities for a variety of implant conditions (e.g., incident ion type, energy, incident angle, and problem geometry).

In the energy range of interest, a few keV to a few MeV incident ions, ion-atom interactions are adequately described as isolated binary encounters with a specified interatomic potential\(^2\). We model two interactions: elastic collisions with atomic nuclei and the inelastic interactions with atomic electrons. The latter can be approximated by a continuous slowing down process without angular deflection. For elastic collisions, which result in large energy transfers and angular deflections, a differential cross section is constructed from an inter-
atomic potential. However, ion cross sections are highly forward-peaked and approach a singularity, making impractical an expansion of the scattering kernel in Legendre polynomials. The Boltzmann Fokker-Planck (BFP) approach gets around this difficulty by representing the forward-peaked component in the Fokker-Planck limit, leaving a smooth large angle kernel that can be expanded in Legendre polynomials. Thus, the equation describing ion transport is

\[
\vec{\Omega} \cdot \nabla \psi(\vec{r}, E, \vec{\Omega}) + \Sigma_s^B(E) \psi(\vec{r}, E, \vec{\Omega}) - \frac{\partial}{\partial E} [S(E) \psi(\vec{r}, E, \vec{\Omega})]
\]

\[
= 2\pi \int_0^\infty dE' \int_4^\infty d\vec{\Omega}' \Sigma_s^B(E' \to E, \vec{\Omega}' \cdot \vec{\Omega}) \psi(\vec{r}, E', \vec{\Omega}')
\]

\[
+ \frac{\alpha(E)}{2} \left[ \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} + \frac{1}{(1 - \mu^2)^2} \frac{\partial^2}{\partial \phi^2} \right] \psi(\vec{r}, E, \vec{\Omega}).
\]  

(1)

where \(\Sigma_s^B(E)\) is the smooth large angle scattering kernel, \(S(E)\) is the stopping power (electronic and restricted nuclear), and \(\alpha(E)\) is the momentum transfer cross section. The MCNP code, which simulates equation (1) for coupled electron-photon transport, has been adapted for ion transport applications. A code named YATC has been developed to compute the cross-section data required by MCNP.

In the following figures, a narrow beam is normally incident on a slab of single element, amorphous material where the deposition profiles are radially symmetric. Figures 1 and 2 compare the results of our methodology against simulations performed with an industry ion transport code called TRIM (which models 1D geometries). Figure 1 compares deposition profiles of 20 MeV aluminum incident on silicon and Figure 2 compares the profiles of 100 keV gold incident on gold. Both ion deposition and energy deposition are depicted in the plots with the energy deposition represented as two curves; the ionization is the energy deposited due to electronic stopping and the energy to recoils is energy deposited by other mechanisms.
Figure 3 illustrates the capability of this methodology to model the radial spread of deposited ions by plotting results of a 100 keV boron incident on silicon simulation. For these problems as well as for other ion-atom pairs at various incident energies, we have observed MCNP results in good agreement with TRIM. We will next extend the methodology by performing ion simulations involving multi-materials and three dimensional heterogeneities.

**Figure Captions**

**Figure 1:** Ion and Energy Deposition of 20 MeV Al into amorphous Si

**Figure 2:** Ion and Energy Deposition of 100 keV Au into amorphous Au

**Figure 3:** Ion Deposition of 100 keV B into amorphous Si

**References**


Ions Deposited per Angstrom per Source Ion

TRIM energy to recoils
TRIM ionization
YATC/MCNP energy to recoils
YATC/MCNP ionization

TRIM ion deposition
YATC/MCNP ion deposition

Energy Deposition [eV/Angstrom]

depth [Angstroms]

0.007 0.006 0.005 0.004 0.003 0.002 0.001 0.000

0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

10^3 10^2 10^1 10^0 10^-1 10^-2 10^-3 10^-4

100.0 200.0 300.0 400.0