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One-Dimensional Ion Implantation Model using Boltzmann Transport Equation

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To apply the Boltzmann transport equation (BTE) to ion implantation, the target material should be divided into a number of small segments Δz as shown in Fig.1. At each depth, the number of particles with energy E_i and traveling angle θ_j is given by a momentum distribution matrix F_{ij} (i=1···i_{max}, j=1···j_{max}). The number of particles transferred to all final states of equal energy but different angles is given by

$$\sum_{j'} \Delta F(ij \rightarrow i'j') = \frac{F_{ij} N \Delta Z}{\cos \theta_j} \int_{T_1}^{T_2} d\sigma_n(T)$$
(1)

where N is the number density of the target material, T_1 and T_2 are the minimum and maximum energy transfers which take a particle from a state of energy E_i to one of states of energy E_i , (< E_i) and $d\sigma_n(T)$ is the nuclear differential scattering cross section.

Eq.(1) is valid only if travel distance of particles, $\Delta z/\cos\theta_{i}$, is small enough so that total scattering probabilities for a particular group of particles does not exceed unity. Allowable step size satisfying the condition described above becomes very small for low energy ion implantation. The step size Az should be a few angstrom for arsenic ion implantation at 50 keV. In order to keep the travel distance of scattered particles in reasonable range, main- and sub- meshes shown in Fig.2 are used at each depth in our new model. А momentum distribution matrix F_{ij} is assigned to each mesh. The particles scattered at depth z are transferred to either the main mesh at the depth, $z + \Delta z$, or the sub-mesh at the same depth, z. Back scattered particles are considered to be stopped at the depth, z, and removed from the mesh because particles scattered toward the sample surface involve large fractional energy loss. After all of the particles in the main mesh are transferred, the role of the main mesh and the sub-mesh at the same depth are exchanged and the calculation is repeated.

The new method described above make it possible to use quite large step size, Δz , compared to the model reported so far without losing accuracy.



Fig. 1 Schematic illustration of a target material.



Fig. 2 Schematic illustration of our new model.