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Molecular Dynamics Simulation of Low Energy Boron and Arsenic Implant into Silicon

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Abstract—We have studied the implantation of boron and arsenic ions into silicon by classical Molecular Dynamics simulation. Single ion implant into the dimer reconstructed *Si*{100}(2×1) surface has been examined at energies between 0.25 keV and 5.0 keV, at both normal incidence and at non-channeling incidence. By using a new model for electronic stopping, developed for semi-conductors and containing only one fitted parameter, we have been able to accurately calculate the depth profile of the implanted *B* and *As* atoms. The results of the calculations are compared to the predictions from a Binary Collision (BC) model for the dopant profile, and to experimental data. This allows us to examine the low energy limits on the validity of the BC approximation, with the aim of producing modifications to the BC model to extend its validity into the sub-keV regime.

I. INTRODUCTION

The use of computer simulation as a method for studying the effects of ion bombardment of solids is now well established. Binary Collision (BC) 'event-driven' codes can be used to accurately calculate such properties as the ranges of implanted species and the damage distributions resulting from the collision cascade within a reasonable computational time. In this type of simulation, each particle trajectory is constructed as a series of repulsive, two-body encounters, with initially stationary target atoms. This allows for efficient simulation, but leads to failure of the method at low energies. When the crystal binding energy is of the same order as the energy of the bombarding species, or when multiple collisions, and collisions between moving atoms are important, the BC approximation is no longer valid.

Molecular Dynamics (MD) simulation uses a far more realistic description of the interaction between atoms. In the case of *Si*, a three-body or many-body potential, rather than a pair potential is required to model the stable diamond lattice, and to account for the bulk crystal properties. Thus, MD provides a more reliable description of the collision processes, but at the expense of a far greater computational requirement.

The calculations described below were carried out to confirm the accuracy of a new model for the electronic energy loss [1], when used for low energy (less than 10 keV) MD simulation of ion implant in *Si*. As the BC approximation is not reliable in this regime, the results offer a way of examining the systematic errors within the BC model, by comparison between the predictions from the two simulation methodologies. Determining the nature of these errors is a first step towards extending the applicability of BC simulations to the 0.1 keV to 5 keV energy range.

II. EMPIRICAL POTENTIAL FUNCTIONS

Interactions between *Si* atoms are modelled by Tersoff's potential [2];

$$E = \tfrac{1}{2}\sum_{i\neq j} f(r_{ij})\left[V_R(r_{ij}) - b_{ij}V_A(r_{ij})\right] \tag{1}$$

where $f(r_{ij})$ is a cutoff function that restricts interactions to nearest neighbours, $V_R(r_{ij})$ and $V_A(r_{ij})$ are Morse-like pair functions of the interatomic separation, r_{ij}, and b_{ij} is a many-body function that can be regarded as an effective Pauling bond order;

$$b_{ij} = \left[1+\zeta_{ij}^{\ \eta}\right]^{-\delta}, \text{ and} \tag{2}$$

$$\zeta_{ij} = \sum_{k\neq i,j} f(r_{ik})g(\theta_{ijk})\exp\left[\alpha\left\{r_{ij}-r_{ik}\right\}^{\beta}\right] \tag{3}$$

where $g(\theta_{ijk})$ is a bond-angle term. Thus b_{ij} incorporates information about the local environment of the bond between atoms i and j. Due to this formalism, the potential can describe features which are very different to the tetrahedral diamond structure, such as defects and surfaces.

The ZBL 'universal' [3] screened Coulomb potential is used to model the ion-*Si* interactions, and in the close-range repulsive part of the Tersoff *Si-Si* potential. The potential energy between two atoms is given as;

$$\begin{aligned} V(r) &= \frac{C}{r/a}\Phi(r/a) \\ C &= \frac{Z_1 Z_2}{a}\frac{e^2}{4\pi\varepsilon_0} \\ \Phi(r/a) &= \sum_{i=1}^{n} c_i \exp\left[-d_i r/a\right] \\ \frac{e^2}{4\pi\varepsilon_0} &= 14.3997 \text{ eVÅ} \end{aligned} \tag{4}$$

where Z_i is the atomic number, e is the charge on an electron, e_0 is the permittivity of vacuum, and a is the screening length, given by;

$$a = \left(\frac{9\pi^2}{128}\right)^{1/3} a_B \left(Z_1^{0.23} + Z_2^{0.23}\right)^{-1} \quad (5)$$

where a_B is the Bohr radius.

The ZBL *B-Si* and *As-Si* potentials are smoothly truncated at a distance comparable to that used in the Tersoff *Si-Si* potential, i.e. at around 1.5 × the sum of the covalent radii of the atoms involved.

The repulsive pair term in Tersoff-type potentials is not sufficiently strong for small atomic separations. To overcome this deficiency, the repulsive term is splined to a shifted ZBL potential, by joining the two functions at the point where they are cotangent. In the case of *Si-Si* interactions, the join is at an atomic separation of 0.69 Å, and requires the ZBL function to be shifted by 148.7 eV. The increase in the value of the short-range repulsive potential compensates for the attractive part of the Tersoff potential, which is present even at short-range.

III. ELECTRONIC STOPPING MODEL

A new model that involves both global and local contributions to the electronic stopping is used for the electronic energy loss [1]. The model contains only one fitted parameter that has the same value for *B* and *As* ions, for all energies and incident directions.

The model was developed for use in a modified UT-Marlowe BC code. One small modification to the model is required to allow its use in MD, due to the fact that an atom is usually interacting with more than one other atom at a time. This modification takes account of multiple contributions to the local electron density, whilst ensuring that the background electron density is only counted once. This is achieved by calculating the one electron radius as;

$$rs = \rho_i^{-1/3} \quad \text{where} \quad \rho_i = \frac{0.119\pi}{0.74} + \sum_{\substack{j \neq i \\ r_{ij} < 1.441\text{Å}}} \left[rslloc_{ij}^{-3} - \frac{0.119\pi}{0.74} \right] \quad (6)$$

where *rslloc* is the one electron radius calculated from the charge density of a single atom, and the constant term is the contribution from the background charge density. This ensures that the damping force is a continuous function of atomic position.

IV. INTEGRATION SCHEME

The paths of the atoms are integrated using Verlet's algorithm [4];

$$\begin{aligned} \mathbf{r}_{n+1} &= \mathbf{r}_n + \mathbf{v}_n \Delta t + \mathbf{a}_n \Delta t^2 / 2 \\ \mathbf{v}_{n+1} &= \mathbf{v}_n + \left[\mathbf{a}_{n+1} + \mathbf{a}_n\right] \Delta t / 2 \end{aligned} \quad (7)$$

As the velocity of the particles varies considerably during a trajectory, a variable timestep scheme is used for the integration. For high energy simulations the potential energy as well as the velocity of atoms is important, as atoms may be moving slowly but have high potential energies during impacts. The timestep is selected using;

$$\Delta t_n = \frac{C_{DIS}}{\sqrt{\max_{i=1,N} \left(\frac{2 \times \left[KE_i + \max(0, PE_i) \right]}{M_i} \right)}} \quad (8)$$

where KE_i , PE_i and M_i are the kinetic energy, potential energy and mass respectively of atom *i*, and C_{DIS} is a constant with a value of 0.05 Å. When the timestep is increasing a weighted sum of the previous and predicted timestep of the form;

$$\Delta t_n' = \tfrac{3}{4} \Delta t_{n-1} + \tfrac{1}{4} \Delta t_n \quad (9)$$

is used, to prevent rapid oscillations in the size of the timestep. During a typical trajectory, the timestep averages about 0.8 fs, with the total energy of the system conserved to 0.03 %.

V. SIMULATION DETAILS

The atomic masses were set to that of the most abundant isotope in each case. The target was 28 Å on a side, and up to 450 Å deep. This required around 24,000 atoms for the largest simulations and resulted in around 95% of incoming ions becoming trapped within the lattice, with 5% passing through the base. At the start of each trajectory an undamaged silicon target was heated to 300 K by giving all atoms appropriate velocities and displacements from their lattice sites. Periodic boundary conditions were applied to the sides of the target, with free boundaries in the vertical direction.

Ions were always incident at random positions over the smallest possible representative area of the surface. The incident direction of the ions was either normal to the surface (channeling case), or at 10° to the surface normal (non-channeling). For the non-channeling case, half the ions had an azimuthal angle of 22° to the surface dimer rows, and half were at an angle of 68° to the dimer rows.

Simulations were run until the total energy of the ion was below 5 eV, at which point it was assumed to be trapped. Around 1000 trajectories were run to generate statistics for each case considered. The simulations were run on 25 SUN & 30 SGI workstations over a period of two months.

VI. RESULTS

Fig 1. to Fig 6. show the calculated concentration profile of the *B* and *As* ions for various incident energies and directions. Also shown are the profiles calculated

using the modified UT-Marlowe BC code [1], and the available Secondary Ion Mass Spectrometry (SIMS) data.

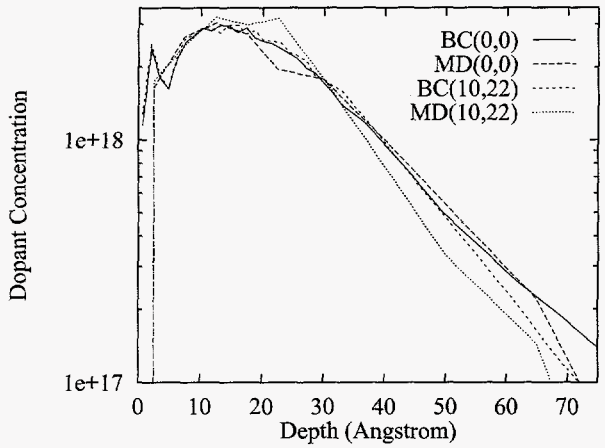

Fig. 1. Implantation profiles for channeling and non-channeling 250 eV *B* calculated using MD and BC.

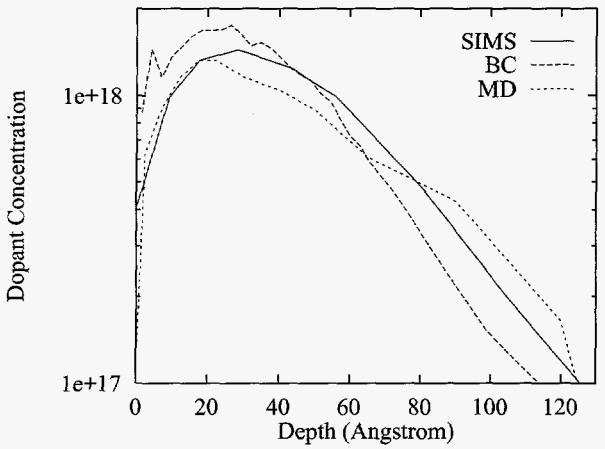

Fig. 2. Implantation profiles for channeling 500 eV *B* measured by SIMS, and calculated using MD and BC.

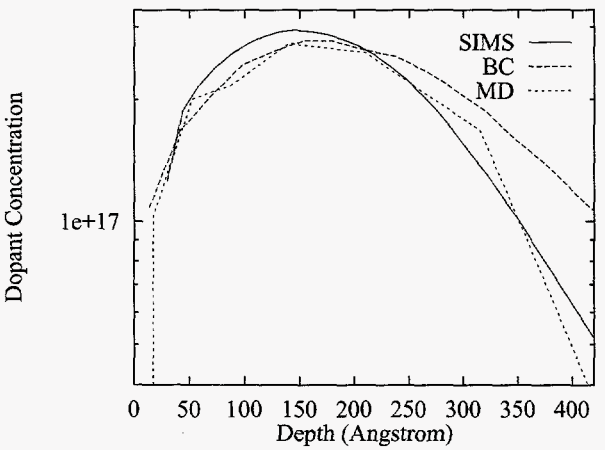

Fig. 3. Implantation profiles for non-channeling 5 keV *B* measured by SIMS, and calculated using MD and BC.

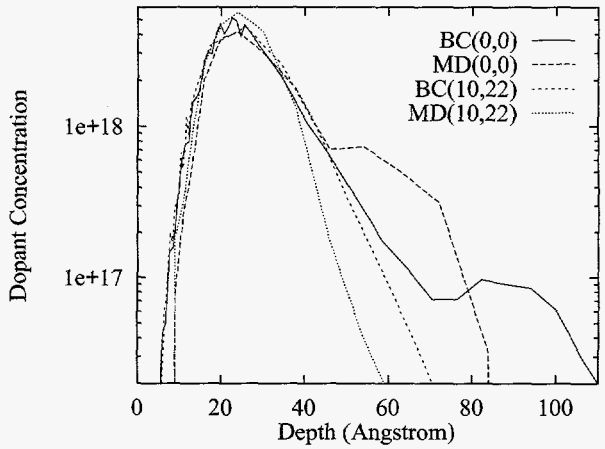

Fig. 4. Implantation profiles for channeling and non-channeling 1 keV *As* calculated using MD and BC.

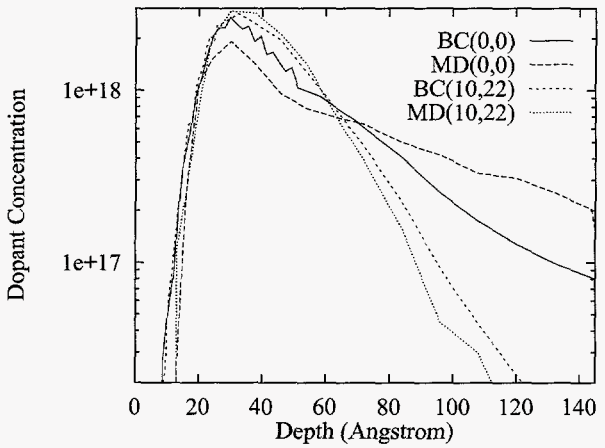

Fig. 5. Implantation profiles for channeling and non-channeling 2 keV *As* calculated using MD and BC.

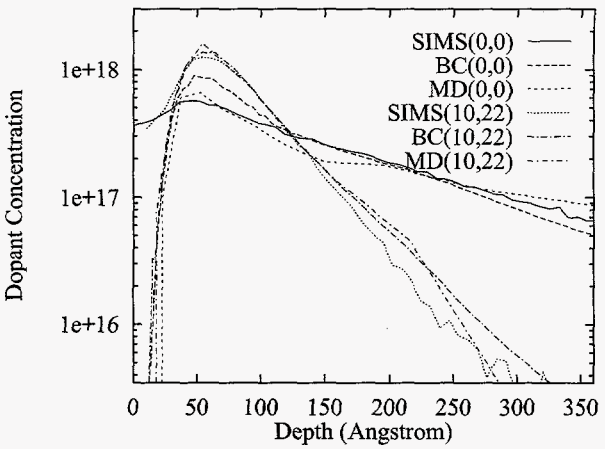

Fig. 6. Implantation profiles for channeling and non-channeling 5 keV *As* measured by SIMS, and calculated using MD and BC.

The results of the MD calculations show very good agreement with the available experimental data, and with

the higher energy (5 keV) BC results. For ion implants at energies of 1 keV and below, there is disagreement between the MD and BC results. This is more evident for the case of the heavier *As* ion than for the *B* ion.

Hence, it appears to be the velocity, rather than the kinetic energy energy of the ion that determines the breakdown of the BC model. The agreement between the two models is better for the non-channeling simulations than the channeling simulations at low energy. This suggests that the lack of an accurate description within the BC model of the 'soft' and multiple collisions that occur during channeling is responsible for much of the discrepancy.

Even at the low energies considered here, the electronic stopping was found to have an important effect on the range of ions in the channeling cases. By examining individual trajectories, it was found that up to 30% of the energy of the ion was lost in this way.

Fig. 7. shows the variation in the damping coefficient, i.e. α, where the damping term due to electronic energy loss is expressed as $\alpha \mathbf{v}$, and $\mathbf{v}$ is the velocity of the ion (α is a function of the ion's velocity, atomic number and its local environment). The figures illustrate typical trajectories at channeling and non-channeling incidence, at 1 keV and 5 keV for both types of ion.

The baseline in these figures corresponds to the ion interacting with the background electronic density, whilst the peaks occur when the ion approaches a *Si* atom and experiences the higher local electron density. There is very little velocity dependence in α at the low energies considered here.

The large dependence of α upon the local atomic environment suggest that models that assume a constant value for this coefficient will ignore much of the physics causing electronic energy loss, and may generate incorrect concentration profiles.

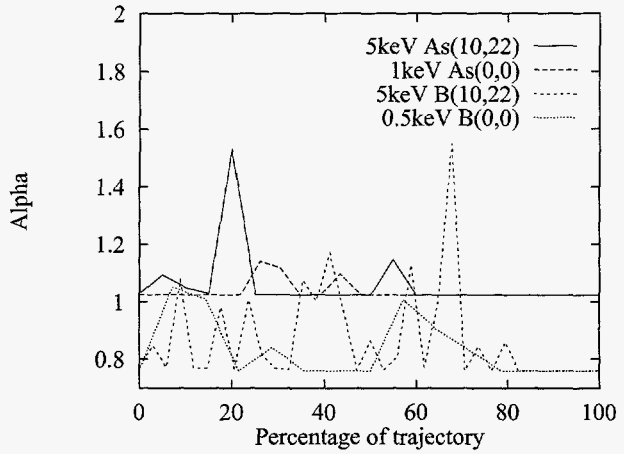

Fig. 7. Changes in the value of the damping coefficient during typical simulation trajectories.

VII. CONCLUSIONS

There is very good agreement between the MD results and SIMS data. The MD model consists of standard empirical potentials developed for bulk *Si* and ion-solid interactions, and the electronic stopping model with only one free parameter fit to intermediate energy (10 keV to 100 keV) SIMS data.

The failure of the BC approximation for low energies was expected, due to the nature of the model used within the calculation. It should however be possible to increase the accuracy of the description of low energy and multiple collisions, using MD results to test and calibrate new collision models.

There is only a small amount of good SIMS data for low energy ion implantation into *Si*. The agreement between MD and the available SIMS data suggests that MD alone may be used to generate data for testing against the low energy BC results when experimental data is not available.

In order to increase the accuracy of the MD results and generate data on the tails of the implantation profiles, larger sets of trajectories are required to reduce statistical errors. This in turn requires a corresponding increase in the efficiency of the computer simulation. This will be obtained by several methods, including variance reduction, the use of multiple timesteps, and by only calculating the paths of atoms directly interacting with the ion.

Another possibility that is now being explored is to systematically 'turn off' components of the MD model. This allows us to examine which parts of the model are essential to produce accurate results and hence should be incorporated into the BC simulations in some way.

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