

Atomistic Simulations of Ion Implantation and Diffusion

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Abstract

Improvements in atomistic simulations have made possible important advances in the understanding of transient enhanced diffusion. In this paper we discuss some of the issues involved in designing a simulator that can handle actual device-processing time and length scales, but also include atomic level detail. We also present a few results from a Monte Carlo simulator of implantation and annealing. Although we concentrate on Monte Carlo modeling, links to more detailed simulations such as molecular dynamics and first-principles methods and to experiments are essential. We discuss the influence of processing conditions, including the dose, dose-rate, and temperature during implantation.

Simulations of the processing of Si devices provide valuable guidance during the design phase for new devices. These models are being improved by including better portrayals of the physical mechanisms and more accurate values of the rates and configuration energies. Although much of this progress has been accomplished using carefully controlled experiments and sample analysis, atomistic models have begun to provide useful information on mechanisms and energies. The maturation of atomistic modeling is largely a result of the increasing power of computers and algorithms, which can now sustain simulations over length and time scales that are sufficient to capture most of the important aspects of Si processing. Our approach is to incorporate new results from these simulations into the continuum simulator PROPHET [1,2], although direct use of these models for device design is also feasible. The combination of atomistic simulations and experiments is very powerful, and the decreasing cost of these simulations makes them more competitive with experiments with each new generation of devices.

Atomistic simulation techniques can be divided into three categories, depending on the level of detail included in the model. Models including quantum calculations of electron distributions (first-principles methods) are the most detailed [3]. They involve a large computational cost, but have the advantage that energies of specific atomic configurations can be calculated directly, without requiring fitting parameters. Although the methods include some uncontrolled approximations, and are limited to small numbers of atoms, direct information on saddle point and binding energies for dopant and point defect interactions is available only through such calculations. Fitting simulations to experimental data may also provide a unique set of atomic interaction energies, provided the experiments are carefully designed. [4].

Classical molecular dynamics (MD) simulations employ empirical force laws which are adjusted to fit a combination of experimental data and first-principles calculations [5]. These methods are much more efficient than those discussed above, since the force law calculation replaces the complex calculations of the electron distribution. Using these

methods, it is possible to simulate systems containing tens of thousands of atoms for nanoseconds or more. This provides sufficient time and space for simulating the energetic collisions of a 5keV Si ion with a Si target crystal, as illustrated in Fig. 1(a). However, it is not possible to simulate the subsequent anneal that is used to reduce the damage and activate the dopant, since this process involves times on the order of seconds.

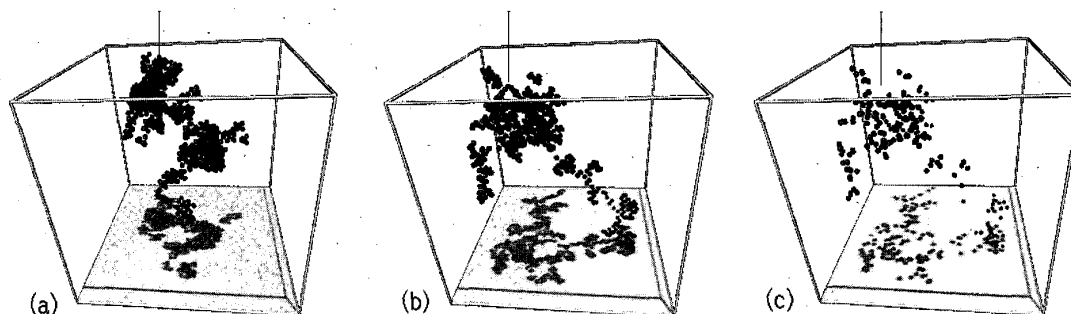


Figure 1. (a) Simulation by MD of the damage caused by a 5keV Si atom colliding with a crystalline Si target. In this case, the computational cell is 13.5nm on an edge, and contains 1.6×10^5 Si atoms. Only atoms of the target with more than 0.2eV of potential energy are plotted. (b) MARLOWE simulation of the same process. Only atoms with more than 0.2eV of initial recoil kinetic energy are plotted. (c) MARLOWE simulation of the same process, but plotting vacancies and interstitials created by the impact.

The comparison in Fig. 1 of MD simulations with the binary collision code MARLOWE shows that the energy distributions created by the two approaches are comparable. After a short anneal, the results annealing the configuration of vacancies and interstitials of the MARLOWE simulations (using a 15eV threshold for a recoiling atom to be able to leave its lattice site and produce a vacancy-interstitial pair) are almost identical with those for full MD. Both approaches yield distributions of vacancies, interstitials, and clusters of these point defects. The two methods do not predict similar results in the case where the dose and energy of the ions are sufficient to generate amorphous layers. The binary collision codes do not account for the damage to the Si target resulting from low energy collisions and local heating in the cascade regions. The original binary collision models describe the damage only in terms of point defects and are not capable of representing amorphous regions. However, as shown in Fig. 1, the sizes of the amorphous regions can be calculated approximately based on the energy distribution calculated from MARLOWE, and we are currently applying this approach to the study of amorphization.

The MC simulator is a hybrid model, using MARLOWE to calculate the damage due to implantation, and a MC diffusion simulation for damage annealing. Transient enhanced diffusion (TED) is calculated in the MC diffusion simulation, using the calculated vacancies and interstitials as illustrated in Fig. 1(c). The coordinates of the vacancies and interstitials are transferred to the MC diffusion simulator, where they are selected for diffusion hops at rates based on their diffusivity. Other events included in the diffusion simulation are: (i) clustering of like point defects, (ii) recombination of vacancies with interstitials, (iii) recombination and generation of point defects at surfaces and interfaces, (iv) evaporation of point defects from clusters, (v) pairing of point defects with dopant atoms, (vi) diffusion of pairs, and (vii) clustering of dopant atoms with point defects. The large number of rates required to simulate these events can often be calculated using MD

and first-principles calculations [3,6], although it is crucial to test the results against actual experiments. The reliability of the rate calculations is not yet sufficient to develop a model based totally on first-principles parameters. Some of the parameters developed using information from calculations and experiments are given in reference 7.

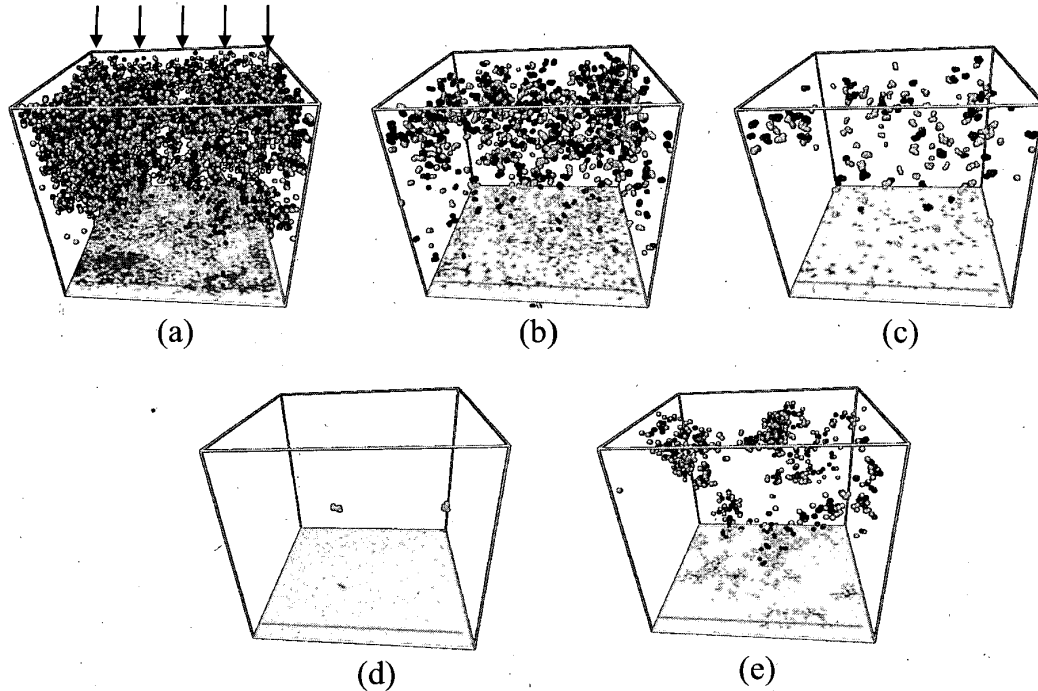


Figure 2. Illustration of point defects simulated for 5keV Si atoms implanted into a Si target. Interstitials are light gray, vacancies are dark gray, and the computational cell shown here is 30nm on an edge, and (a)-(d) are for a $1 \times 10^{13}/\text{cm}^2$ dose. (a) Point defects remaining at the end of the implantation process at 300K, (b) after aging at 300K for 1 hour, (c) after annealing at 1100K for 10-3 sec, (d) after annealing at 1100K for 0.5 sec, and (e) after implantation of a $1 \times 10^{12}/\text{cm}^2$ dose of 5keV Si.

The simulation of an implant is accomplished by alternating the implantation of an atom with the MC diffusion process, with the time of the diffusion determined by the dose rate of the implant. Figure 2 (a) shows the point defects at the end of a $1 \times 10^{13}/\text{cm}^2$ implant simulation, and (b) –(d) show the results during later stages. After the 0.5sec anneal at 1100K shown in (d), the recombination events have left only a few interstitial clusters, resulting from the net interstitial excess due to the implanted ions. The high concentrations of point defects in the very early stages have been reduced dramatically due mainly to recombination of Frenkel pairs. At doses of $1 \times 10^{13}/\text{cm}^2$ and higher, the results of the model are consistent with the “+1” model, which postulates that rapid recombination will eliminate the Frenkel pairs at such an early stage that only the interstitial corresponding to the implanted ion will contribute significantly to TED.

However, at lower doses the Frenkel pairs can make an important contribution to TED [8]. Figure 2 (e) shows the point defects immediately after implantation with a dose of $1 \times 10^{12}/\text{cm}^2$, and it is apparent that recombination of the vacancies and interstitials from Frenkel pairs may be less efficient than for higher doses due to the larger spacing between point defects. Indeed, the MC simulations show that this is true, and Fig. 3 gives some results for a range of implant doses. These results evaluate TED from the number of times

an interstitial visits a site in the target lattice for an anneal to completion. It applies to an interstitial diffuser such as B, and is a measure of the number of opportunities for a substitutional B atom to pair with a Si interstitial. Note that the contribution per implanted ion increases by a factor of 20 for very low doses, and the “+1” model greatly underestimates the expected amount of TED.

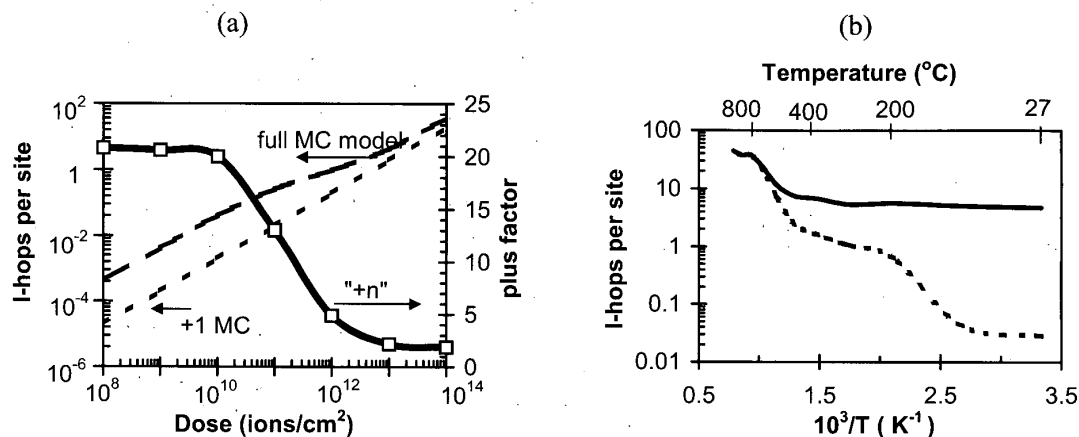


Figure 3. The number of times an interstitial visits a site in the target is plotted in (a), for 10keV implants. The dashed curve corresponds to the simulation of the MC model with all Frenkel pairs included, whereas the dotted curve is the result of a modified MC model with only the interstitial corresponding to the implanted Si atom, as implied by the “+1” model. The ratio of the number of site visits for full damage to that for the “+1” approach is given by the solid curve and the right axis. The site visits for high temperature implants are given in (b); the solid curve giving the number of visits after an implant and an 1100K anneal, and the dashed curve giving the number for an implant alone.

In conclusion, we have found that the additional detail of the atomistic models has provided the ability to simulate diffusion phenomena for a wide range of conditions, and we expect these models to find increasing use in the development of accurate process simulations.

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