Simulations of Ion Beam Induced Damage in Silicon: Coupled Kinetic Monte Carlo and Molecular Dynamics Simulations

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Introduction

Damage formation during ion implantation is a complex process that cannot accurately be modeled by binary collision simulations alone. Molecular Dynamics (MD) simulations are an accurate method to simulate ion implantations at low temperatures. However, because lattice vibrations have to be resolved by the MD time steps, MD cannot simulate thermally activated processes at time scales that occur in industrial processing steps. On the contrary, kinetic Monte Carlo simulations (kMC) consider only events that change the structure of the crystal. Due to this fact, it is possible to treat thermal processes with kMC. Nevertheless, kMC cannot handle ballistic processes because the binding and formation energies of complex defect clusters are often unknown. However, both ballistic and thermally activated processes need to be taken into account in order to predict the amount and types of defects depending on the implant parameters, such as ion species, energy and temperature. To combine the advantages of both simulation methods we have introduced and tested a coupling scheme of MD and kMC. Doing this, one has to be careful not to lose too much information of the coordinates and of the kind of defects when transforming them from one scheme to the other. Otherwise, complex defects cannot be restored in MD any more once they have been transformed.

Scheme of Coupling

We couple binary collision (BC)/MD and kLMC simulations. The BC calculations are used to generate the initial recoils for the MD simulations. Details of the binary collision program IMSIL can be found in [1] and the description of the MD scheme is given in [2], [3]. As input for the lattice kinetic Monte Carlo (kLMC) simulation, physical quantities like formation and binding energies of point or extended defects are required, which we take from ab-initio simulations [4] – [8]. The crucial point in coupling MD and kMC simulations is to minimize the loss of information about the defects by caused by their transformation them from MD to kMC and vice versa. We achieve this using the following scheme. First, we identify the defects generated in MD. The atom positions are analyzed with respect to spheres centered on ideal lattice sites with radii equal to half the nearest neighbor distance in the ideal lattice. If a sphere contains no atom, the lattice position is labeled as a nearest-neighbor-sphere (NN) vacancy. If an atom is outside all of the spheres, its position is labeled as NN interstitial. When transforming the kLMC defects to the MD scheme one obtains only nearest neighbor (NN) defect immediately, but not atoms that are shifted less than half the nearest neighbor distance from their lattice sites. However, such defects are generated if the MD cell including the NN defects is relaxed. We tested the stability of defects and almost the whole damage (96% ± 2.2%) is reproduced.

Results

To demonstrate the coupling we examine the differences in the damage generation for the implantation of heavy and light ions at room temperature. As heavy ion, we have chosen arsenic and as light ion, boron. We have performed a BC simulation of a 1 keV As ion and put the generated recoils into a MD simulation. After 5 ps the MD simulation is stopped and the identified NN defects are transformed to the kLMC model. The kLMC simulation is performed until all single vacancies have disappeared leaving only two main clusters, which are transformed back to MD and relaxed for 5 ps. In the next step, another As cascade which overlaps partly with the first cascade is simulated. The cluster generated by the first cascade has shrunk in the final defect configuration due to a recrystallization initiated by the recoils of the second cascade. As a second example, we have implanted 1 keV boron ions into silicon. We produced a predamaged crystal by a coupled BC/kLMC simulation. We implanted a dose of $5\times10^{14}/cm^2$, which caused about 4% of the lattice atoms to be displaced. The damage was transformed to MD and relaxed. Another boron cascade has then been simulated with MD in the predamaged crystal, and the additional damage has then been compared with the damage produced by a boron cascade generated by the same primary recoils in an undisturbed crystal. In the undisturbed cascade, the boron implantation generated 20 NN defects, in the predamaged cascade 12 additional defects, indicating a sublinear increase in damage concentration.

Conclusion

A scheme of coupling kLMC with MD has been introduced, which allows an almost complete reconstruction of MD clusters once they have been transfomed to kLMC. With this coupling, both the quenching of collision cascades and the thermally activated processes can now be considered in one simulation.

Acknowledgements

This work was sponsored in part by the Austrian Science Fund, Project No. 15872-N08.

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