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Temperature effect on damage generation mechanisms during ion implantation in Si. A classical molecular dynamics study

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Abstract. We have studied the temperature effect on the damage generation mechanisms in silicon, suppressing the influence of dynamic annealing. We have done dedicated classical molecular dynamics simulations to determine how the ballistic mechanism and the thermal spikes are affected by temperature. We have quantified the minimum energy required to permanently displace an atom from its lattice position by a ballistic collision. We have found that the displacement energy threshold does not change appreciably with temperature. However, when subthreshold energy is simultaneously deposited in several neighboring particles in a finite volume, i.e. when thermal spikes occur, there is an enhancement of the generation of damage with increasing temperature. In high energy recoils both mechanisms are combined, and it results in an increase of the generated damage with temperature.

Keywords: Damage generation, Ion implantation, Cold implants, Silicon, Temperature effect, Molecular dynamics.
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INTRODUCTION

Nowadays cold implants are being incorporated into the fabrication process of electronic devices [1]. Ion implantation at low temperature facilitates the creation of amorphous layers at the Si substrate [2]. This permits to take advantage of the high substitutional fraction of dopants reached during solid-phase epitaxial regrowth of the amorphous layer. To achieve the desired performance of fabricated junctions an optimal control of implant conditions, temperature among them, is required. In addition, the damage generation by energetic collisions in the Si lattice plays an important role in other applications such as Si radiation detectors, which operate at cryogenic temperatures. In radiation detectors, defects generated by incoming radiations increase the leakage currents, change the effective doping concentration, and reduce the charge collection efficiency [3, 4].

Implant temperature has two main effects on the damage generated. It affects the recombination and diffusion of defects. These phenomena are thermally activated and thus they are enhanced as temperature increases, effect known as dynamic annealing. In addition, the generation of damage itself might also depend on temperature. Damage generation by energetic collisions can be regarded as a combination of two basic mechanisms: a ballistic mechanism and thermal spikes [5]. Atoms of the substrate that receive an energy transfer larger than the displacement energy threshold, E_d, can initiate a subcascade, leaving behind a vacancy and generating a self-interstitial when they stop. This energy transfer can come from the ballistic collision with an implanted dopant, or as a consequence of the interaction with energetic α, β, or γ radiations. For Si, theoretical estimations for E_d range from 10 to 30 eV [6]. Damage generated through these ballistic displacement events can be described in terms of pairs of vacancies and Si self-interstitials, called Frenkel pairs. When a number of neighboring atoms receive individually an energy bellow the displacement energy threshold, but enough energy is deposited in all the neighboring atoms (i.e. thermal spikes) amorphous regions can be generated through the local melting of the lattice [7]. Thermal spikes are especially relevant as the energy of implanted dopants and recoils decreases, which results in multiple interactions with target atoms.

In this study we have analyzed how temperature affects the damage generation by energetic collisions. We have used dedicated classical molecular dynamics (CMD) simulations for this purpose. First, we have quantified separately how the temperature modifies the basic damage generation mechanisms. Then, we have analyzed the damage generated by high energy recoils, where the energy transfer to the substrate results in a combination of ballistic displacements and thermal spikes. It is worth noting that our study only takes into account the damage generation itself, i.e. the displacement of atoms due to energetic interactions between moving atoms and lattice atoms, and not the

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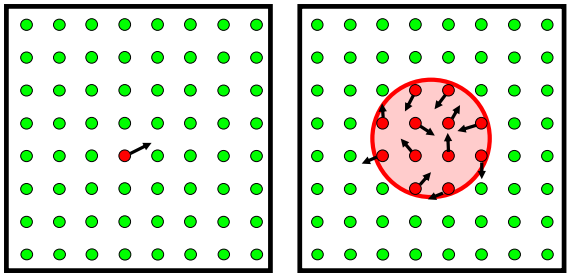

(a) Isolated recoils (b) Group of energetic atoms

FIGURE 1. Schematic representation of the initial conditions used in our CMD simulations for (a) isolated recoils and (b) thermal spikes.

temperature driven dynamic annealing that takes place after the pure damage generation process is over.

SIMULATION DETAILS

We performed our CMD simulations at temperatures between 0 K and 300 K. We used the Tersoff 3 [8] empirical potential to describe the Si-Si interactions. This potential has been previously used to study ion irradiation in Si and provides and adequate description of this process [9, 10].

We first studied the effect of temperature on the energy displacement threshold, E_d. For this purpose a randomly-selected atom of the simulation cell was given certain amount of kinetic energy with velocity in a random direction, as it is schematically represented in Fig. 1.a. Initial kinetic energies of these isolated recoils were chosen between 10 and 50 eV, and simulation cells contained ~14000 atoms. To analyze the effect of temperature on the damage generated by thermal spikes, we used the procedure described in detail in Ref. [7]. In short, a number of atoms located in a sphere in the center of the simulation cell were given a certain kinetic energy between 0 and 20 eV/atom with velocities in random directions. This is schematically represented in Fig. 1.b. We considered several groups of initially excited atoms, containing 60, 80 and 100 atoms. Simulation cells had ~130000, ~160000, and ~200000 atoms, respectively.

Finally we studied the combined effect of both mechanisms by simulating individual recoils of 1 keV of nuclear deposited energy of B, Si and Ge into Si. Recoils were initiated at the center of the simulation cell with velocity in random direction. Energy losses due to the interaction between the ion and the electrons were not considered. Thus, the initial energy of ions was completely deposited in the target. Simulation cells contained ~340000 atoms. In these simulations the Tersoff 3 potential was splined to the repulsive ZBL pair potential [11] at short distances to properly describe the ion-Si high energy interactions.

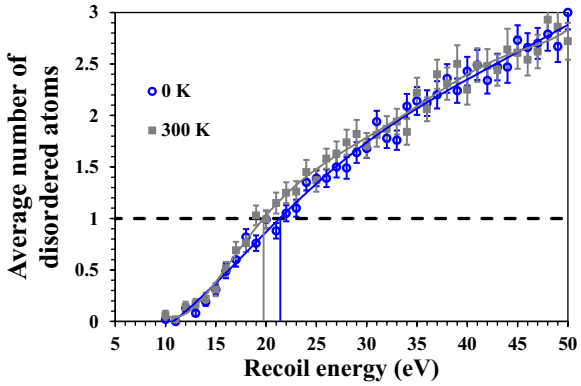

FIGURE 2. Average number of disordered atoms as a function of the recoil energy for isolated low energy recoils at 0 K and 300 K. Lines are to guide the eye.

In all the performed simulations we run a total of 100 simulations for each set of initial conditions in order to improve statistics. We used cubic simulation cells and periodic boundary conditions were applied in the three spatial directions. The size of the simulation cells was enough large to assure that interaction among moving atoms due periodic boundary conditions was avoided, and that the temperature increase once the deposited energy was spread through the cell was lower than ~30 K in all the cases. It is worth noting that dynamic annealing was prevented since the total simulated time of our simulations was at the scale of picoseconds, much shorter than the characteristic time constant of dynamic annealing in Si that is of the order of ms [12].

Defects and damage zones generated through the simulation cell were identified using a method based on the time average of atom coordinates [13]. This method has been successfully employed to identify defects and damaged regions in Si [14-16]. It consists on performing a time average of atom coordinates over 1000 time steps once the energy deposited into the cell was dissipated throughout the cell. This procedure eliminates thermal vibrations and provides the local equilibrium positions for all atoms. Then, averaged atomic coordinates are compared with the original perfect lattice positions. When an atom is closer than 0.7 Å to a lattice site the atom is associated to that site, otherwise it is labeled as *disordered atom* (DA) therefore contributing to damage.

SIMULATION RESULTS AND DISCUSSION

The average number of disordered atoms as a function of the recoil energy in the simulations where the energy is given to isolated recoils is represented in

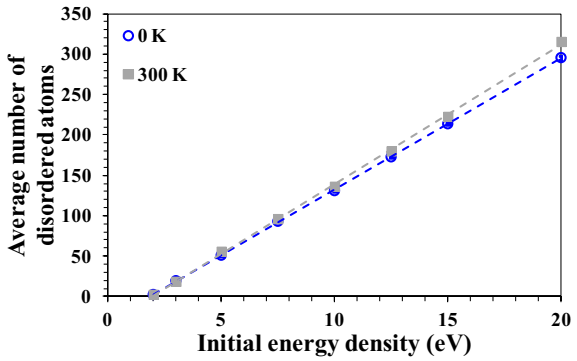

FIGURE 3. Average number of disordered atoms as a function of the initial energy density for groups of 60 initial excited atoms at 0 K and 300 K. Error bars are hidden by symbols. Dashed lines are linear fits of data.

Fig. 2. It can be seen that for the considered temperatures, 0 K and 300 K, the number of disordered atoms increases as the initial recoil energy increases. A very similar trend is followed for both temperatures. There is some difference in the region were one disordered atom is obtained, but the difference is within the error bars.

The final average number of disordered atoms generated by groups of energetic atoms as a function of their initial energy density is represented in Fig. 3 for the case of 60 initial energetic atoms. Simulations show that the amount of generated damage increases linearly with the initial energy density for the temperatures considered, and there is a slight damage generation enhancement at 300 K with respect to 0K. Equivalent results were obtained for the cases of 80 and 100 initial energetic atoms (not shown).

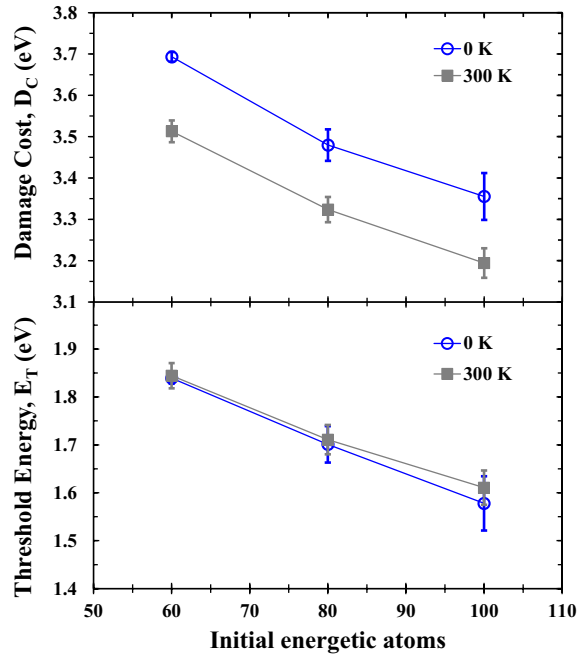

FIGURE 4. Energy density threshold, E_T, and damage generation cost, D_C, for 60, 80 and 100 initial energetic atoms at 0 and 300 K.

The final number of disordered atoms, N_{DA}, can be fit to the expression

$$N_{DA} = \frac{N \cdot \rho - N \cdot E_T(N)}{D_C(N)} \qquad (1),$$

where ρ is the average energy density (in eV/atom), N is the initial number of atoms that receive energy, and $E_T(N)$ and $D_C(N)$ are the *threshold energy density* for damage production, and the *damage generation cost*, respectively [5]. These parameters can be understood as follows. E_T represents the minimum energy density necessary to reach an initial metastable disordered state. Nevertheless, the influence of the surrounding crystal lattice can drive disordered atoms to back to perfect lattice positions. In order to keep atoms permanently disordered, or at least a fraction of them, an additional amount of energy is required. D_C controls the final number of DA that are generated with the remaining energy.

The values of the parameters E_T and D_C obtained for the different groups of initial energetic atoms considered are shown if Fig. 4. It can be seen that both E_T and D_C decrease with the initial number of energetic atoms, i.e. the collective motion at the energy spikes for larger groups of energetic atoms make it easier to reach the metastable disordered state. Temperature hardly has any effect on E_T, but D_C is lower at 300 K than at 0 K. Consequently, the damage generation due to thermal spikes is enhanced with temperature.

The combined effect of the ballistic mechanism and thermal spikes takes place in high energy recoils. In table 1 we summarize the amount and characteristics of the damage generated in the recoils of 1 keV of B, Si and Ge in Si at 0 K, 150 K, and 300 K. We observed that, for a given ion type, the total amount of disordered atoms increases with temperature. The relative increment of the number of generated DA with respect to 0 K, i.e. (N_{DA}(T) – N_{DA}(0K))/N_{DA}(0K), is nearly independent of the ion type. Regarding the morphology of the generated damage, we found that, for a given ion type, the average and the maximum defect size increase with temperature, i.e. not only more damage is generated as temperature increases, but also larger defects are generated. Since the ballistic mechanism of damage generation is not affected by temperature, this enhancement appears to be related to thermal spikes occurring during recoils. The larger defects also indicate that the enhancement on damage generation observed in recoils is due to local thermal spikes.

In the case of the implantation process for the fabrication of electronic devices, the temperature

effect analyzed in the present study will affect heavy ion and molecular implants since thermal spikes are especially relevant in these cases. In the case of radiation detectors, when incident radiation only produces single displacement events, for example for neutrons and electrons with an energy above ~180 eV and ~260 keV, respectively [3, 4], the amount of Frenkel pairs generated in the lattice will not change if temperature increases. However, in the case that Si recoils are produced, for example for neutrons and electrons with energies above ~35 keV and ~8 MeV, respectively [3], the enhancement on damage generation with temperature due to thermal spikes can boost the degradation of the detector.

Our simulations show that damage generation during energetic collisions is enhanced as temperature increases. This apparently contradicts experimental findings. As we mentioned previously, we did not take into account dynamic annealing, which takes place once the damage generation phase is over. Dynamic annealing drives the diffusion and recombination of generated defects, and therefore their concentration at the end of the implantation process. From the comparison of our simulation results with experimental findings we can conclude that the enhancement of damage generation is overcome by dynamic annealing. The net balance is that damage accumulates more easily as temperature decreases since generated defects are more stable.

TABLE 1. Summary of the total number of disordered atoms (DA), average defect size, and average maximum defect size in the recoils of 1 keV of B, Si and Ge in Si at 0 K, 150 K, and 300 K.

	0K	**150K**	**300K**
Boron			
Total number of DA	65.9	70.7	74.5
Average defect size	9.9	11.0	12.3
Maximum defect size	16.5	18.6	20.5
Silicion			
Total number of DA	82.1	86.6	93.0
Average defect size	24.6	28.5	32.5
Maximum defect size	34.2	39.9	43.9
Germanium			
Total number of DA	109.0	114.3	123.0
Average defect size	66.2	71.6	78.3
Maximum defect size	76.1	82.1	89.9

CONCLUSIONS

In conclusion, we found that the displacement energy threshold does not change with temperature, i.e. single displacements generated by isolated atomic collisions are not affected by temperature. However, there is an enhancement in the generation of damage with temperature when thermal spikes occur. As a consequence, recoils initiated in the lattice are more effective generating damage as temperature increases, and generated defect are more complex. Then, the pure damage generation in silicon due energetic collisions is enhanced with temperature. Nevertheless, experimental findings indicate that this enhancement is overcome by dynamic annealing, and damage is more effectively accumulated at lower temperatures.

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