Molecular Dynamic Simulations of Ion Induced Damage in Silicon

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Molecular dynamic simulations are performed by us to aid binary collisions model development of both simple defects and amorphous pockets and for a quantitative comparison with RBS/C measurements.

The molecular dynamics simulations are done with the program MDSWV, which has been provided by Konrad Gärtner from the University of Jena. It is based on the Stillinger-Weber potential and uses the Verlet algorithm for time integration with an adaptive step. An atom in the center of the MD cell has been kicked in a random direction with an energy from 5 to 80 eV. The final state of the MD cell has been compared with the ideal lattice and the displaced atoms have been examined.

The molecular dynamic cell consists of $10 \times 10 \times 10$ unit cells (8000 atoms). Periodic boundary conditions in x and y directions and a fixed bottom and top layer in z-direction have been chosen. The temperature was set to 300 K. The simulations lasted approximately 2.5 ps. After about 1 ps there was no significant change in the final configuration of the displaced atoms

To identify a displaced atom the following criterion has been applied: An atom is considered to be displaced if the probability that its deviation is caused by the lattice vibration is under 10^{-6} (assuming a Gaussian distribution around the ideal lattice site). Calculations yield that for a temperature of 300 K an atom is displaced if it has a distance above 0.44 Å from the ideal lattice site.

To separate interstitials, vacancies, bond, and other defects from atoms which are displaced from their lattice site by the forces of the neighboring defect, another criterion has been applied. It is based on spheres centered on ideal lattice sites defined by the undisturbed lattice. If the sphere contains no atoms, the lattice position is labeled a vacancy. An atom that has no free lattice site in the sphere centered at the atom position (i.e. there are no lattice sites in the sphere or only lattice sites that are occupied by nearer atoms) is labeled an interstitial. The radius of the sphere is set equal to half the next neighbor distance.

In the observed energy range mainly Frenkel pairs, bond defects and di-interstials could be found, also several clusters with three interstitials (about 3% of the number of the Frenkel pairs). Greater amorphous pockets could not be created in this energy range (see Fig. 1). Clusters with more than two interstitials are very seldom and therefore are not included into the statistics. Additionally it can be seen that the defect distribution is much less than those of the Kinchin-Pease approach.

The interstitials have been investigated with respect to their structure. 90% of the generated Frenkel pairs are split-interstitials. The rest are tetrahedral interstitials.

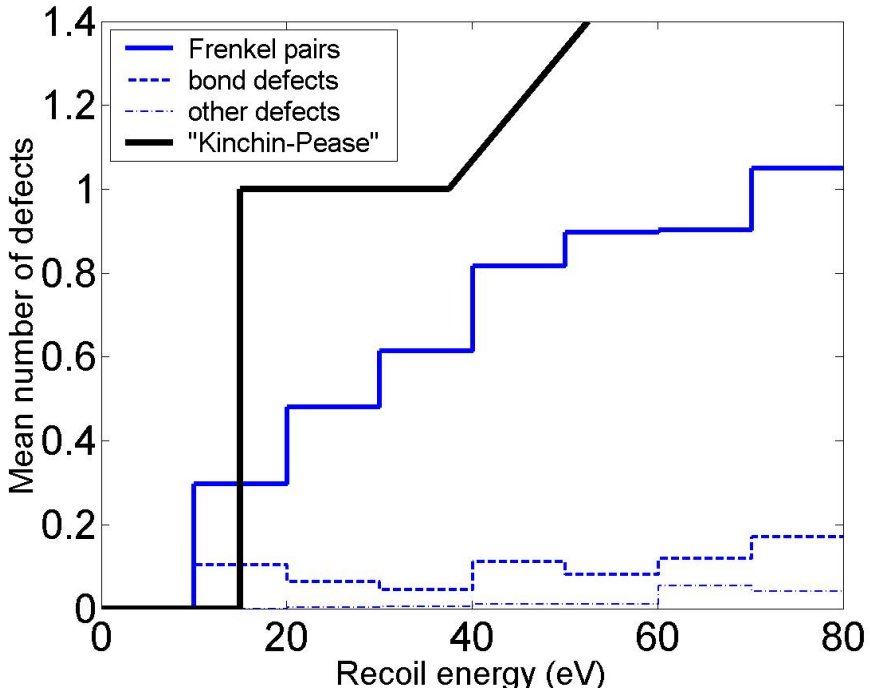

Fig. 1: Mean number of Frenkel pairs and other effects per recoil event and “the modified Kinchin-Pease” model.

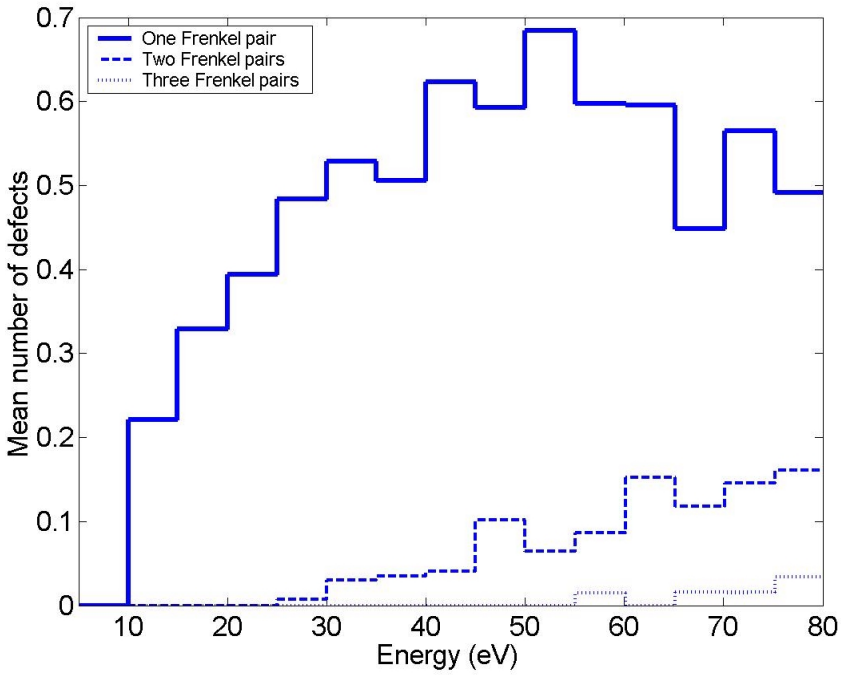

Fig. 2: Probability that 1, 2, or 3 Frenkel pairs are generated in a recoil event.

Figure 2 shows that in most cases exactly one Frenkel pair is generated. But at higher energies the proportion of the cases in which more than one Frenkel pair is generated

increases. That in this energy range most Frenkel pairs have an I-V separation below 9.2 Å is shown in Fig. 3.

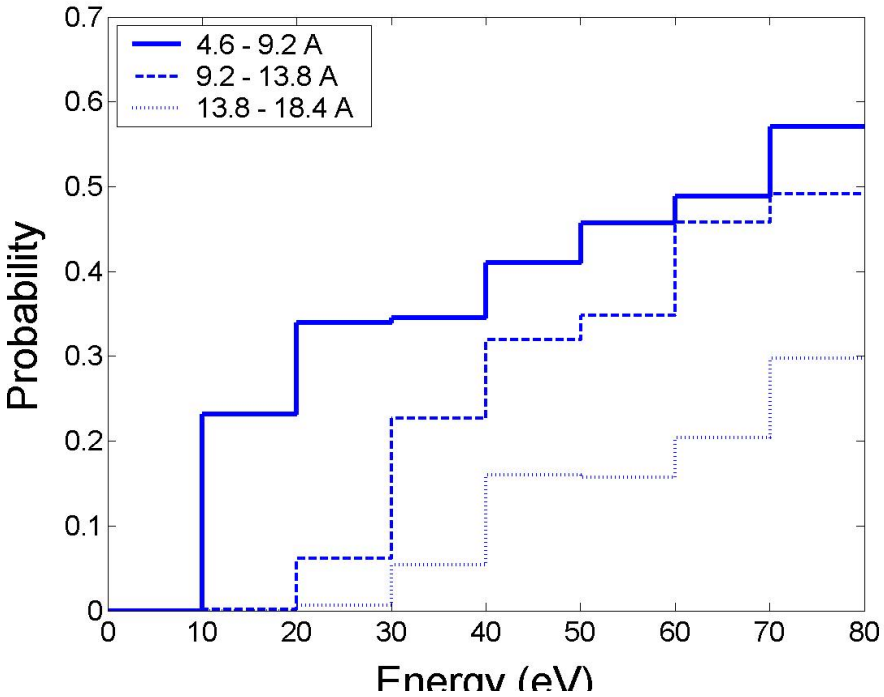

Fig. 3: Probability that a Frenkel pair with distances between I and V in the given ranges is generated in a recoil event.