A STUDY OF POINT DEFECTS IN CRYSTALLINE AND AMORPHOUS SILICON

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ABSTRACT

The point defects in crystalline and non-crystalline state of tetrahedrally bonded semiconductors show both common features and differences. The case of crystalline and amorphous silicon is discussed. The single point defect and small clusters of point defects are analyzed on the basis of a simulated crystalline lattice and amorphous network of silicon.

Keywords: Semiconductors, Amorphous silicon, Point defects, Modeling

The defects in solids have important consequences on their properties. The silicon wafers are now used in ultra low scale integration (ULSI) of the semiconducting devices and for solar cells

[1]. On the other hand amorphous silicon thin films are more and more used for various purposes: for the fabrication of light sensors or photovoltaic elements and other new devices as e.g. diodes with ultra thin absorber [2]. The correct working of the devices both in crystalline and amorphous form, the lifetime of devices and the stability of their properties depend in many cases on the native or induced defects in the basical material.

[2]. The single crystalline wafer of silicon show deviations from the perfect crystalline lattice, as dislocations, point defects (Schotky and Frenkel) and impurity atoms. Recently it was shown that a new type of defect is favorable from the energetical point of view: the so-called deformon state.

[3]. This state is realized by reversing the position of two atoms in the crystalline lattice by changing the system of bonds without introducing dangling bonds in the system. Nevertheless, the free energy of the lattice shows a moderate increase.

As opposite to the case of crystalline silicon, the ideal amorphous silicon consists in a continuous random network of atoms, that exhibits only short-range order, i.e. the first coordination sphere of every atom is preserved, although some deviations from the ideal tetrahedral bonding are produced. There was demonstrated by modeling an ideal crystalline lattice that a great number of deformons introduced in the lattice transforms the lattice in a network that shows many similarities with the amorphous silicon [4].

This short communication reports the effects induced by point defects and small clusters of point defects on the overall local distortion in a crystalline and in amorphous silicon, with the aim to evidence the particularities of the structural modifications related to defects in completely different network of atoms, either ordered or disordered (amorphous).

The modelling was performed in the frame of a Monte-Carlo – Metropolis method, for the search of the minimum free energy, in models of crystalline silicon and amorphous silicon (continuous random network) [5]. Two models have been used: an array of crystalline silicon with 300 simulated atoms and a model of non-crystalline silicon with 2052 atoms.

The generation of a point defect in crystalline silicon has been followed by energy relaxation. The energy relaxation was performed in the frame of the valence force field model as developed by Keating [6], with the force constants for silicon published by Martin [7]. The final configuration, either in the case of single defect (hole) or multiple defects was determined.

Table 1 shows the results obtained by simulation. For the sake of accuracy, the simulation was applied, also, to a piece of crystalline silicon with 300 atoms. It is remarkable that the hole produced into a perfect silicon lattice does not induce significant structural changes around the defect. The lattice remains stable. Two neighboring defects or small cluster of defects behaves similarly. In the case of amorphous silicon the positions of the vicinal atoms around the void formed by the expulsion of a silicon atom are significantly modified as a consequence of network relaxation. In fact, the amorphous network is locally stressed, and, therefore, by

eliminating some atoms it is possible to get a new state of lower free energy. Table 1 shows the values of the structural parameters in the crystalline lattice and in amorphous silicon network before and after the elimination of one, two, and five atoms. In all the cases an energetical relaxation of the lattice (network) was carried out in the frame of a Monte Carlo-Metropolis procedure, in order to reach the stable configuration of minimum free energy.

Table 1. Structural parameters related to point defects in crystalline and amorphous silicon as obtained by defect simulation.

Structural Parameter	Point defects in cryst. Silicon (Model; 300 atoms)			Point defects in amorphous silicon (model: 2052 atoms)			
	Cryst.	1 void	2 voids	Amorph	1 void	2 void	5 voids
Distance, r_1 (nm)	2.35	2.346	2.345	2.348	2.348	2.341	2.359
rms (r1) (nm)	0.0	0.005	0.005	0.063	0.067	0.057	0.067
Angle, ϑ (deg.)	109.469	109.469	109.469	109.86	109.818	109.591	109.321
rms (ϑ)	0.0	0.000	0.000	8.3248	8.4698	8.6547	8.2614
Dihedral angle (deg.)	60.0	59.80	59.78	59.50	59.51	59.46	59.49
2-nd distance, r_2 (nm)	3.830	3.830	3.830	3.857	3.866	3.859	3.874
rms (r_2) (nm)	0.0	0.000	0.000	0.244	0.245	0.250	0.303

The effect of the radiation (especially nuclear particle radiation) on the structure of both crystalline and amorphous materials is very important for the applications in cosmic space. The semiconducting devices based on silicon play a leading role in the modern electronics and in silicon detectors for nuclear radiation. The point defects are produced by high-energy particles. In the case of point defects some change in the hybridization of the silicon atoms that surrounds the defect (hole) is possible. Khohlov and Mashin have shown [8] that there are not limitations in principle for the existence of elemental silicon consisting of atoms that there are not in the sp3 hybridization state.

The bulk damage in silicon detectors caused by hadrons or higher leptons, respectively gammas, is primarily due to displacing a primary knock on atom (PKA) out of its lattice site. The threshold energy for this process is ~25 eV. Such single displacements results in a pair of silicon interstitial and a vacancy (Frenkel pair) can be generated by e.g. neutrons and electrons with an

energy above 175 eV and 260 keV, respectively. Low energy recoils above these thresholds energy will usually create point defects. For recoil energies above ~ 5 keV a dense agglomeration of defects is formed at the end of the primary PKA track. Such disordered regions are referred to as defect clusters [9]. In the case of the radiation damage caused by Co-60 gammas (maximum energy of Compton electrons is only 1 MeV) cluster production is not possible and the damage is exclusively due to point defects. The strategy used up to day for improving the radiation tolerance of silicon is the adequate defect engineering [10].

Defect engineering involves the deliberate addition of impurities in order to reduce the radiation-induced formation of electrically active defects. It was found that that oxygen plays a significant role for improvement of the radiation tolerance, while carbon has an adverse effect. The role-played by the oxygen and carbon was modeled and discussed by Lazanu et al. [11].

In other materials, as e.g. chalcogenide glasses, the defects produced by irradiation are more complex and depend on the dimensionality and the composition of the glass [12].

Point defects in crystalline and amorphous silicon 347 A point defect induced in the non-crystalline or amorphous silicon behaves differently from the case of crystalline silicon. The distortion around the void induced by the elimination of an atom from its place is very small. Thus, the crystalline lattice is locally stable (see Table 1). Even two neighboring defects do not destabilizes the lattice around them.

The general problems of the non-crystalline solid structures were discussed, recently, by Popov [13]. Two main types of models for non-crystalline solids from the category of tetrahedrally bonded semiconductors have been developed. In the first type of models the network is of the type continuous and random. No dangling bonds are permitted. This is the case of the model used in our calculations. In the second group of models, several domains of the first type are interconnected and, as a consequence at interface boundaries are more disordered and dangling bonds occur. The detailed structure of the last complex network was studied in the frame of a model with two domains (amorphites) [14, 15].

The importance of having a particular model in the investigation of the effect of the radiation was pointed out by Balberg [16], which provided the first evidence that the crystallites encapsulating tissues in microcrystalline Si: H is different from that of the grain boundaries in polycrystalline silicon and that of the homogeneous amorphous Si: H.

Due to the different system of bonding in tetrahedrally bonded semiconductors and the chalcogenide solids, the behavior of the two types of materials is quite different. Nevertheless, the common feature seems to be the reducing of bond distortion around the void created by the ejection of an atom and the increase of local distortion of the bonds. In both materials the tendency is to eliminate as much as possible, the dangling bonds formed during particle -atom interaction in the process of irradiation.

The network relaxation is very important in the non-crystalline configuration of silicon atoms due to the presence of a high amount of stress in the material. The voids give the possibility to relax the stress. The decrease of stressed state is larger for the case of big holes produced in the network by particle irradiation. As a consequence, the amorphous material subjected to irradiation changes the structure towards a more stable one. From the practical point of view the amorphous silicon must be firstly irradiated in order to reach a state of stability and, thereafter, to be used in the semiconducting devices aimed for working in radiation environment. As regarding the crystalline silicon it could be concluded that only damaging by high fluency of radiation gives an important structural instability, having as a consequence the alteration of the electro-physical properties.

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