The Role of Incomplete Interstitial-Vacancy Recombination on Silicon Amorphization

Luis A. Marqués, Lourdes Pelaz, Jesús Hernández and Juan Barbolla
Departamento de Electrónica, Universidad de Valladolid
E.T.S.I. Telecomunicación, Campus Miguel Delibes, 47011 SPAIN
lmarques@ele.uva.es

Abstract

We investigate the role that point defects and interstitial-vacancy pairs have on the Si amorphization process using molecular dynamics techniques. We show that accumulation of interstitial-vacancy pairs in concentrations of 25% and above lead to homogeneous amorphization. We identify very stable defect structures, consisting of the combination of the pair and Si self-interstitials, which form when there is an excess of interstitials or by incomplete interstitial-vacancy recombination in a highly damaged lattice. These defects could survive long enough at room temperature to act as embryos for the formation of extended amorphous zones and/or point defect clusters.

1 Introduction

The study of the ion irradiation induced amorphization of Si is of particular interest due to the use of increasingly high ion implantation doses in the microelectronics industry. Experiments show that amorphization starts near the ion end-of-range [1] where lattice damage and a net excess of Si interstitials coexist [2]. It has been proposed that the excess interstitials could have an influence on the amorphization process, perhaps through their interaction with the lattice defects created by the irradiation or by forming interstitial clusters that would act as amorphous embryos [3]. This idea has been also suggested to explain the recently achieved amorphization of Si by electron beams [4]. On the other hand, Tang *et al.* proposed that the lattice defect known as *IV pair* could be responsible for the silicon amorphization process [5]. Using molecular dynamics techniques, we have studied the amorphization produced by IV pair accumulation in an attempt to develop a microscopic model to be included in the atomistic diffusion code DADOS [6].

2 The IV pair

The IV pair consists of the atomic bond rearrangement displayed in Fig. 1. The bond lengths obtained from our simulations using the Tersoff 3 potential [7] are in very good agreement with Tight Binding [5] and *ab initio* [8] results, as can be deduced from inspection of Table 1. The obtained formation energy, 3.01 eV, compares with the 3.51 eV from Tight Binding [5] and the 3.26 eV from *ab initio* calculations.

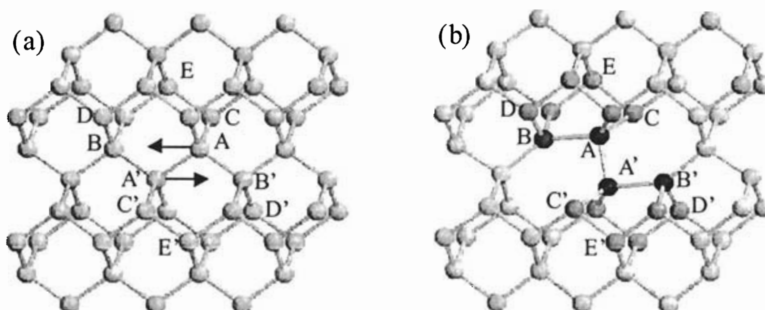

Fig. 1. Formation scheme of the IV pair. Atoms A and A' switch their bonds with atoms B and B'. Darker tones correspond to higher potential energies.

Table 1. Lengths of the bonds involved in the IV pair, expressed in Å. Letters refer to the corresponding atoms in Fig. 1(b).

Bond	This work (T3)	TBMD [5]	*Ab initio* [8]
A-A′	2.28	2.28	2.27
A-B	2.51	2.46	2.46
A-C	2.35	2.38	2.39

We have also studied the stability of the IV pair by computing its time for recombination at different temperatures. The results are shown in the Arrenhius plot of Fig. 2. Extrapolating at room temperature we find a lifetime of only 3 μs, which is too short for the IV pair to survive between successive cascades and thus act as the embryo for Si amorphization, unlike it was proposed previously [5,8].

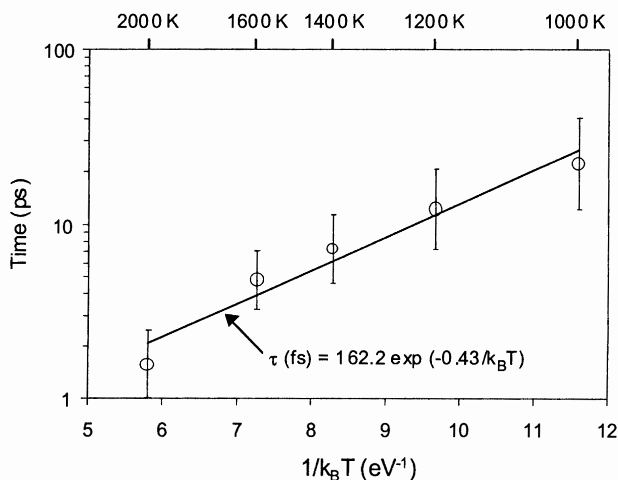

Fig. 2. Arrenhius plot of the time needed for I-V recombination. The line is the best fit to the data, which determines an activation energy of 0.43 eV.

3 Amorphization simulations

In Fig. 3 we display the evolution of the potential energy per atom in samples with different concentrations of IV pairs at several temperatures. As can be seen, samples with concentrations of 10 and 20% recrystallized for all the simulated temperatures. However, samples with 30% of IV pairs remained amorphous. Interestingly enough, the behavior of the sample with a concentration of 25% depends on temperature. After introducing 25% of IV pairs some traces of crystallinity are left. These crystal seeds grow at lower temperatures, but thermal agitation at higher temperatures dissolve them. Consequently, for each temperature there exists a critical damage concentration that prevents recrystallization.

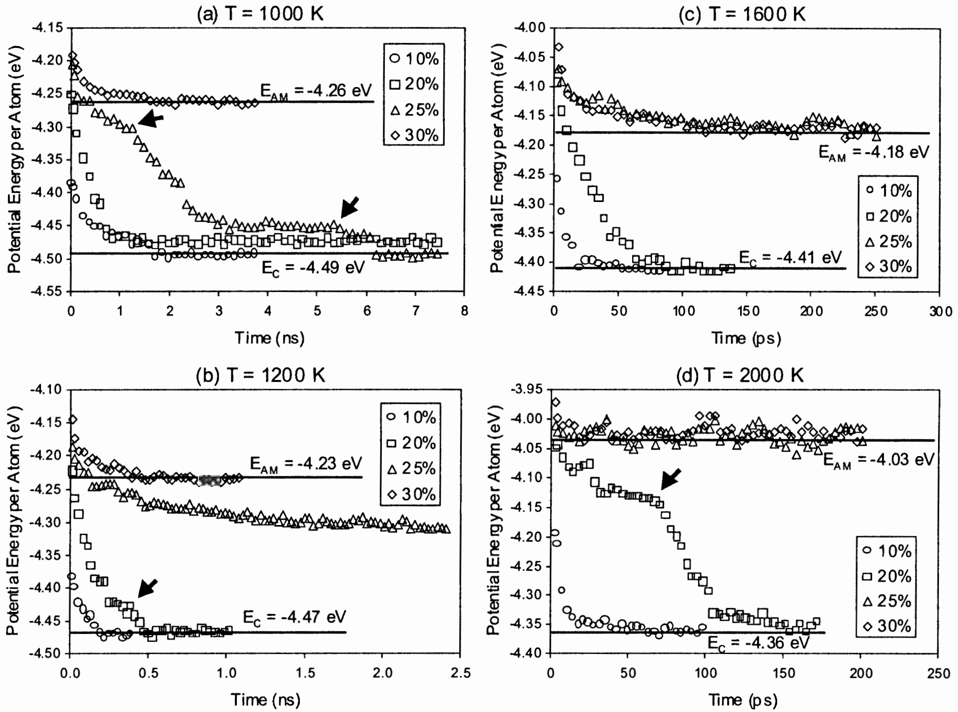

Fig. 3. Time evolution of the potential energy per atom in samples with different IV pair contents during the annealing at several temperatures. Solid lines indicate the mean potential energy per atom in amorphous and crystal Si at each temperature, E_{AM} and E_C, respectively.

For a concentration of 10% energy decay is exponential, and corresponds to an activation energy of 0.45 eV, very close to the barrier obtained for IV pair recombination. This means that 10% is a concentration so low that IV pairs do not interact with each other, and thus the overall crystallization behavior is the same that when there is just one IV pair. However, for higher concentrations the evolution of the potential energy per atom shows plateaus followed by steep decreases, indicated by arrows in Fig. 3. In those cases, IV pairs interact with each other and form more stable structures. The crystallization then implies the collective movement of several atoms which produces a sudden decrease in the potential energy per atom.

4 The IV+2I complex

In our simulations we found very stable defects formed by the combination of an IV pair and two interstitials, shown in Fig. 4(a). We observed that this defect, that we will refer to as *IV+2I complex*, is mobile. Its displacement takes place following the scheme depicted in Fig. 4. This defect can remain stable in the lattice after more than 10 ns at 1000 K, which implies a lifetime at least two orders of magnitude longer that that of the IV pair. This fact means that self-interstitials can stabilize the lattice disorder represented by the IV pair. If the disorder survives between successive cascades, it could accumulate and eventually lead to amorphization. The formation of these complexes is favored when excess of interstitials coexists with the lattice damage, as in the case of ion irradiation. They can also be formed with no net excess of Si self-interstitials if high enough density of IV pairs is present, as in the case of electron irradiation at high doses and low temperatures.

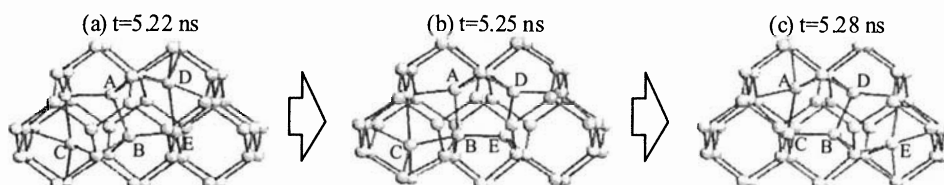

Fig. 4. Atomic pictures showing the time evolution of the IV+2I complex formed during the annealing at 1000 K of the sample with a initial IV pair concentration of 20%.

References

[1] Maszara, W.P., Rozgonyi, G.A. (1986): Kinetics of damage production in silicon during self-implantation. J. Appl. Phys. 60: 2310-2315

[2] Holland, O.W., White, C.W. (1991): Ion-induced damage and amorphization in silicon. Nucl. Instrum. Methods Phys. Res. B 59/60: 353-362

[3] Seidman, D.N., Averback, R.S., Okamoto, P.R., Baily, A.C. (1987): Amorphization processes in electron- and/or ion-irradiated silicon. Phys. Rev. Lett. 58: 900-903

[4] Takeda, S., Yamasaki, J. (1999): Amorphization in silicon by electron irradiation. Phys. Rev. Lett. 83: 320-323

[5] Tang, M., Colombo, L., Zhu, J., Diaz de la Rubia, T. (1997): Intrinsic point defects in crystalline Si: Tight-binding molecular dynamics studies of self-diffusion, interstitial-vacancy recombination, and formation volumes. Phys. Rev. B 55: 14279-14289

[6] Jaraíz, M., Pelaz, L., Rubio, E., Barbolla, J., Gilmer, G.H., Eaglesham, D.J., Gossmann, H.J., Poate, J.M. (1998): Atomistic modeling of point and extended defects in crystalline materials. MRS Symp. Proc. 532, MRS Spring Meeting, San Francisco, pp. 43-53

[7] Tersoff, J. (1988): Empirical interatomic potential for silicon with improved elastic properties. Phys. Rev B 38: 9902-9905

[8] Cargnoni, F., Gatti, C., Colombo, L. (1998): Formation and annihilation of a bond defect in silicon: An *ab initio* quantum-mechanical characterization. Phys. Rev. B 57: 170-177