Self-interstitial trapping by carbon complexes in crystalline silicon

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By combining model-potential molecular-dynamics simulations and *ab initio* calculations we investigate the microscopic mechanism of silicon trapping by carbon substitutional defects (C_S). We find that, upon silicon trapping, carbon is converted into an interstitial mobile complex (C_I) by an efficient exothermic reaction. Interstitial carbon C_I may further interact either with another C_S, forming the well-known C_IC_S dicarbon complex, or with extra silicon and carbon interstitials. In particular, we identify and characterize two structures, namely, C_II and C_IC_I. They are found energetically stable so that they could play a crucial role in the process of carbon aggregation. According to our calculations C_IC_I may be formed by the interaction of one I with a C_IC_S, proving that the latter is not a deactivated trap for interstitials. Our results further suggest that C_II and C_IC_I are seeds for further carbon aggregation.

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I. INTRODUCTION

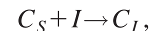
Ion implantation is the standard procedure adopted in silicon bulk processing to place selected dopant populations and profiles into a bulk sample. Due to the release of kinetic energy of the implanted ions to the lattice, a large amount of native point defects is typically created under the ion bombardment. Such defects, in turn, interact with implanted dopant atoms originating a very complex hierarchy of phenomena that affect the overall microstructure evolution of the silicon sample.

Within the above scenario, the case of boron implantation in crystalline silicon is either paradigmatic and technology relevant. On the one side, the full understanding of the temperature-induced evolution of boron doping profiles requires a quantitative modeling of the atomic-scale interactions among dopant atoms and lattice defects. On the other side, it is experimentally well known that boron experiences anomalous transient enhanced diffusion (TED) upon thermal annealing in the presence of an excess concentration of silicon self-interstitials. Accordingly, an undesirable broadening of boron concentration profiles is observed.

Several methods have been proposed so far to control and reduce boron TED, among which is the incorporation of substitutional carbon in silicon.[1] Due to carbon's high efficiency in trapping silicon self-interstitials, the reduction of boron TED in C-rich silicon samples has been experimentally proven. This important result, however, did not represent an ultimate solution to the problem. As a matter of fact, boron TED is only reduced, but not completely suppressed. Furthermore, a decrease in the electrical activation of boron is observed in C-rich implanted samples. Accordingly, the coexistence of C and B in the same lattice region turns out to be detrimental for the overall electrical properties of the sample.

Recently, Napolitani *et al.*[2] have proposed a procedure aimed at a complete suppression of boron TED by silicon self-interstitial trapping in a spatially separated C-rich layer. The key idea is to interpose a C-rich silicon layer between the region damaged by the ion beam and the implanted B profile. The flux of silicon self-interstitials from the damage is in fact filtered and eventually damped by the C-rich layer, thus leaving the B profile nearly unaffected. In this configuration no detrimental effects on B electrical activation were observed.

The current understanding of C-induced quenching of boron TED is based on the occurrence of two different mechanisms: (i) carbon diffusion and (ii) silicon self-interstitial trapping. As for the basic kick-out mechanism providing C diffusion[3,4] it is known that a mobile silicon self-interstitial (I) is captured by an immobile substitutional carbon (C_S) defect. This reaction gives rise to the formation of a new complex consisting of one Si atom and one C atom sharing the same lattice site. Such a complex is usually referred to as interstitial carbon (C_I) and is highly mobile. The C_I complex was experimentally identified by Watkins and Brower,[5] and its migration path was theoretically modeled by Capaz *et al.*[6] The I trapping is then described as a pairing reaction in which a mobile C_I binds to another C_S forming an immobile complex labeled C_IC_S.[7–11] Overall, the effect of carbon on silicon self-interstitial trapping is described by the combined set of elementary reactions



$$C_S+I\rightarrow C_I,$$

$$C_S+C_I\rightarrow C_IC_S. \qquad (1)$$

The concept of C_IC_S carbon pairing, as well as the elementary reactions leading to its formation, has been extensively used in the literature in mesoscopic modeling based on rate equations[12,13] and kinetic Monte Carlo calculations[14,15] to explain the presence of immobile carbon.[16] Nevertheless, it is still unclear whether the picture summarized by the reactions appearing in Eq. (1) is a complete and faithful description of all the possible interactions among C_S, C_I, and I defects. In particular, we need to understand whether all the relevant trapping mechanisms have been indeed considered, as well as investigate the possible formation of C-Si complexes other than C_IC_S. Both features would be of great relevance for developing a more fundamental understanding

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of the microstructural evolution of a C-rich silicon layer where an excess concentration of self-interstitials is present.

In this work we investigate, by a combined approach of model-potential molecular-dynamics (MD) and *ab initio* calculations, the formation of carbon complexes resulting from the interaction of up to two interstitial silicon atoms with a background of carbon substitutional defects in a silicon crystalline environment. We find that (i) silicon and carbon interstitials are highly reactive defect species with a tendency to aggregate by exothermic reactions; (ii) $C_I C_S$ is just one among many other defects formed by the interaction of C_I with its environment; (iii) the carbon complexes considered in this work always tend to grow by capturing interstitial carbon and silicon atoms.

The paper is organized as follows. We first discuss the relevant details of the theoretical framework used in this work (Sec. II). The carbon complex features and their formation mechanisms are discussed in Sec. III. Finally, we draw a comprehensive picture about the possible implications of present findings on the thermodynamics of the system, making use of the experimental evidence in the literature (Sec. IV).

II. COMPUTATIONAL METHOD

The investigation of carbon-silicon interactions and formation of C-Si complexes is a difficult and computer-demanding task that can hardly be studied within the same framework. Therefore we developed a methodology based on a combination of model-potential MD simulations and *ab initio* calculations. Two basic questions must be addressed when investigating any possible binary reaction between defects: (i) Do the two defects attract each other? (ii) Which is the most stable structure of the complex they form?

In order to answer the first question we evaluate the capture (interaction) basin associated to the reaction. We placed one defect at the center of the simulation cell. Then we assigned to each lattice site (on the bond chain starting from the defect) a label, counting the number of steps along the chain joining the defect and the selected site. To limit our investigation to a reasonable number of configurations we restricted ourselves to the bond chains oriented along the $\langle 110\rangle$ and $\langle \bar{1}10\rangle$ directions. The capture basin was then determined by computing the binding energy of the given defect system at different values of the corresponding reaction coordinate. This procedure (see, for instance, Fig. 1) in fact defines the proper reaction direction and reaction coordinate for the selected binary defect-defect coupling. Binding energy is set to zero when the two defects form a noninteracting pair. The binding energy has been evaluated both by an *ab initio* and a model-potential calculation: the latter is useful since it allows for the determination of the basin shape up to distances larger than those accessible by a first-principles approach.

Molecular-dynamics calculations were carried out on a cubic supercell containing 512 atoms. As for the interatomic potential we used the Tersoff multicomponent potential given in Ref. 17. The equations of motion were integrated by a velocity-Verlet algorithm and, due to the light mass of carbon atoms, we used a time step as small as 0.5 fs. We performed structure relaxations based on a standard damped dynamics optimization scheme and simulated annealing. The simulated annealing runs were performed in the *NVT* ensemble implemented on the velocity rescaling thermostat.

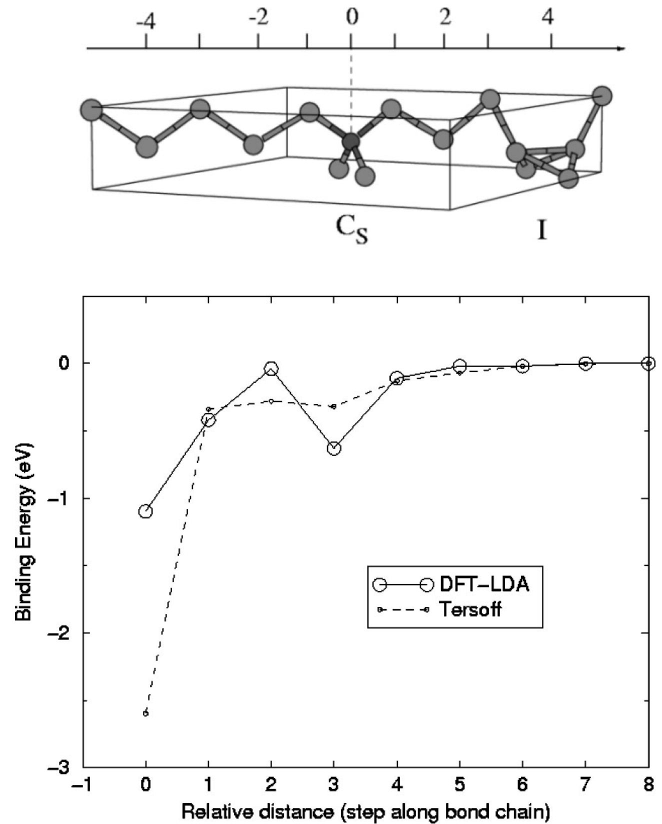

FIG. 1. Top panel: a substitutional carbon C_S atom and a silicon interstitial I interacting along the $\langle 110\rangle$ reaction direction. Black: C; gray: Si. Bottom panel: attraction basin between I and C_S.

As for first-principles calculations, they have been worked out within the local-density-functional-theory pseudopotential framework as implemented in the VASP code.[18] Ultrasoft pseudopotentials[19] provided with VASP were used both for Si and C. Defects are simulated in periodic boundary conditions via the repeated supercell approach. We used cubic supercells containing 216 atoms of linear dimension 16.17 Å. A plane-wave basis set with a kinetic-energy cutoff of 160 eV was used. Our convergence tests showed that the error bar on the relative energies of the defects here studied is ~0.1 eV. We restricted the Brillouin-zone sampling to the Γ point only.

III. STRUCTURE, ENERGETICS, AND FORMATION MECHANISM OF SILICON-CARBON COMPLEXES

In this section we focus on the nucleation of neutral carbon defects in *c*-Si originating from C_S and I interactions. These defects evolve through a set of binary reactions. We limit our analysis to the simplest reactions relevant for the discussion on carbon aggregation in *c*-Si reported in the following section.

A. C_I formation and structure

The carbon interstitial defect originates as the outproduct of the interaction between a silicon interstitial atom and a substitutional carbon by a "kick-out" capture mechanism. In Fig. 1 (top panel) we represent the I and C_S pair along the $\langle 110 \rangle$ direction. According to a well-established picture,[20] we select the lowest-energy configuration for a neutral interstitial Si to be the $\langle 110 \rangle$ dumbbell configuration. The reaction coordinate for I-C_S pairing is defined by the peculiar migration path of the dumbbell: it converts to a tetrahedral interstitial defect at the next position along the $\langle 110 \rangle$ direction and then it moves back to a dumbbell configuration at the second-nearest-neighbor lattice site with respect to the starting position.[20] The attraction basin for the above reaction is reported in Fig. 1 (bottom panel) where it is apparent that model-potential MD simulations qualitatively reproduce the *ab initio* results. In particular, both calculations prove the occurrence of a precapture mechanism (a local minimum in the curve of the energy) when I and C_S are at a distance of three bond lengths. The absolute minimum in energy is reached when the dumbbell and the carbon bind together forming an interstitial carbon split. It is interesting to notice that the attraction basin extends over several bond lengths.

The Tersoff potential correctly reproduces the geometry of the C_I interstitial but overestimates its binding energy. In this configuration C and Si atoms are displaced along the $\langle 001 \rangle$ direction sharing a lattice site. This split is the most stable configuration for C_I in silicon and it is consistent with previous findings.[5,8]

B. Formation of the $C_I C_S$ complex

The C_I defect is a mobile species that can easily diffuse at the typical annealing temperature. After diffusion it may be captured by a substitutional carbon atom forming a dicarbon complex. This structure has been identified experimentally[7] and it is called $C_I C_S$. According to Capaz *et al.*[9] there exist two almost energetically degenerate configurations for the $C_I C_S$ complex (labeled A and B in Fig. 1 of Ref. 9). We compared the energies of the two configurations using a first-principles approach: we find the A variant to be favored over configuration B by 0.4 eV. Recently a third dicarbon complex was estimated,[21] where two carbon atoms are displaced along the $\langle 001 \rangle$ direction. However, our first-principles calculations predicted a formation energy for such a configuration 0.2-eV higher than the A variant of the $C_I C_S$ defect. Therefore in this work we consider this one to be the actual configuration for such a complex.

At variance with the previous case, the interaction energy depends both on the relative distance and on the defect orientation. In Fig. 2 (top panel) we show the two bond chains driving the C_S defect towards the C_I complex and the calculated attraction basin for $C_I C_S$ pairing (middle and bottom panels). The middle panel of Fig. 2 shows the binding energies computed for the C_S approaching the C_I along the upper chain. We see that both model-potential and first-principles calculations predict the existence of a small energy barrier for the recombination of the carbon pair. However they provide a remarkable different binding energy at a close $C_I C_S$ distance. This case represents a configuration where two carbons are first neighbors along the $\langle 111 \rangle$ direction, similar to that found by Liu *et al.*[21] According to present *ab initio* results the corresponding defect complex is energetically unfavored.

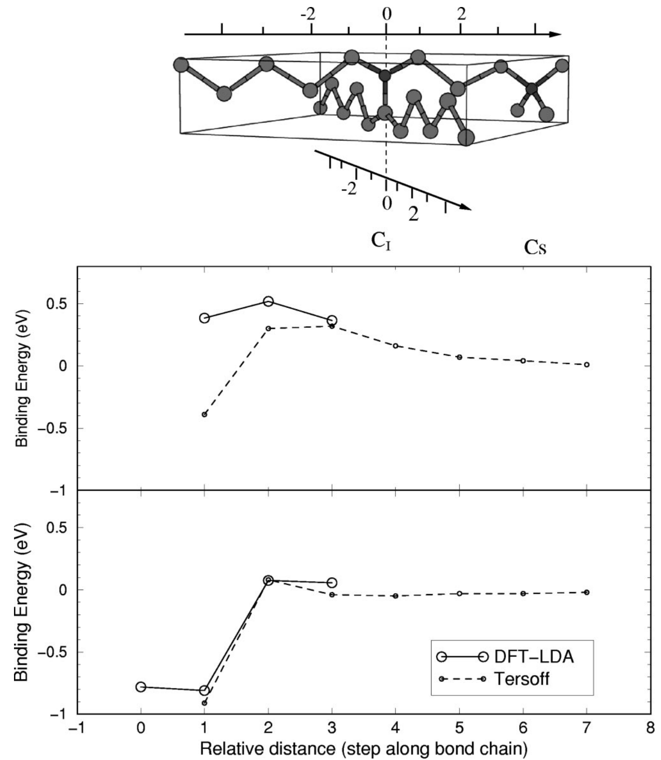

FIG. 2. Top panel: an interstitial carbon atom C_I and a substitutional carbon atom C_S interacting along the $\langle 110 \rangle$ reaction direction (upper chain) or along the $\langle \bar{1}10 \rangle$ reaction direction (lower chain). Black: C; gray: Si. Bottom panels: Attraction basins between C_I and C_S defects along $\langle 110 \rangle$ (middle panel) and $\langle \bar{1}10 \rangle$ (bottom panel) directions.

Figure 2 (bottom panel) shows the binding energies of the C_S-C_I pair when C_S is approaching C_I along the lower bond chain. In this case the recombination is nearly barrierless and the attraction basin does not extend very far away from the C_I defect. Both calculations predict energetically unfavored (positive binding energy) intermediate configurations, providing a binding energy for the $C_I C_S$ complex as large as 0.8 eV.

C. Formation of the $C_I C_I$ complex

We further extend our investigation to consider the capture of an extra silicon self-interstitial atom by $C_I C_S$. The corresponding reaction coordinates and the binding energies are shown in Fig. 3. Let us consider the motion of I along the upper bond chain displayed in Fig. 3 (middle panel). The interaction is strongly attractive with the presence of a precapture process similarly to the C_S-I pairing case. In Fig. 3 (bottom panel) we show instead the energetics computed along the lower bond chain. The key feature is the attitude of the $C_I C_S$ to capture I mobile defects, forming a pretty stable complex that should be considered a precursor for a next

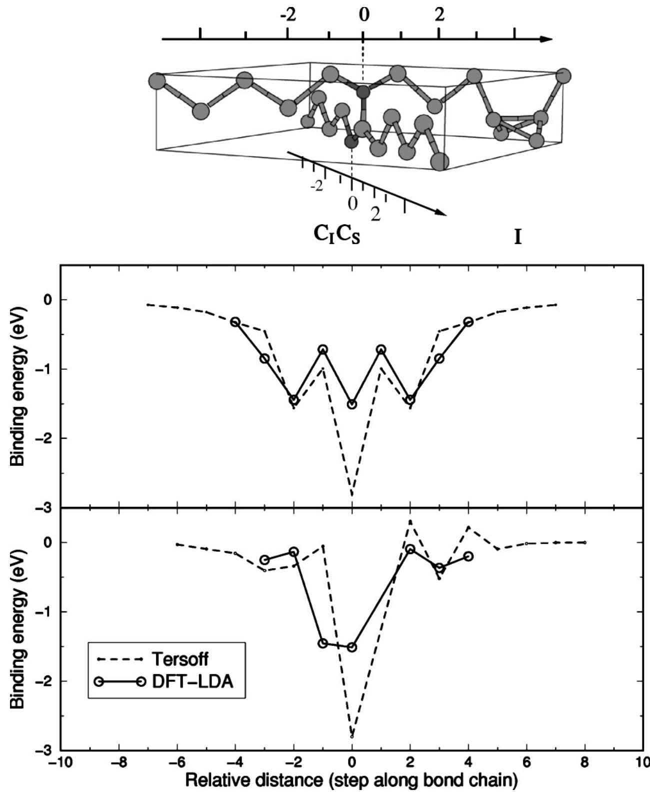

FIG. 3. Top panel: the C_IC_S complex and a silicon interstitial I interacting along the $\langle 110 \rangle$ reaction direction (upper chain) and $\langle \bar{1}10 \rangle$ reaction direction (lower chain). Black: C; gray: Si. Bottom panels: Attraction basins between a C_IC_S complex and a silicon interstitial I along $\langle 110 \rangle$ (middle panel) and $\langle \bar{1}10 \rangle$ (bottom panel) directions.

evolution step. Since the binding energy is as large as 1.5 eV, present calculations clearly indicate that within a supersaturated environment of self-interstitial silicon atoms, C_IC_S represents just an intermediate step of a process leading to the formation of larger complexes.

So far we have not discussed the structure of the defect formed by the C_IC_S-I interaction. Since the attraction basin is characterized by a precapture minimum, it is reasonable to suppose that many different and nearly isoenergetic configurations could be indeed formed as a result of the capture process. To verify the existence of those metastable configurations we performed a thorough simulated annealing search for local minima. After the annealing, most of the estimated input structures (where an I defect was placed close to a C_IC_S complex) came out to be tightly bound, with binding energy ranging from 1.5 to 2.1 eV. The corresponding morphologies are quite similar and closely resemble the same structure: a pair of Si-C dimers where a carbon atom of the first dimer is bonded to the silicon of the second one. Hereafter, we refer to such a defect—represented in Fig. 4(b)—as the C_IC_I complex.

An independent way to obtain such a complex consists of directly simulating its formation at finite temperature. MD simulations confirmed that C_IC_S captures the silicon interstitial forming a thermodynamically stable complex. This result makes us confident about the reliability of the picture drawn

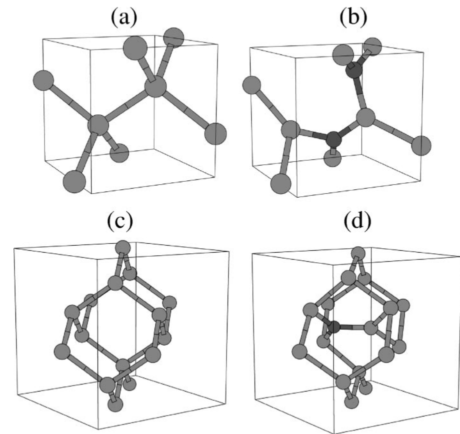

FIG. 4. Lowest-energy configuration of the C_IC_I (b) and C_II (d) defects, compared to the ideal silicon lattices (a) and (c), respectively. Black: C; gray: Si.

in this section. We note that C_IC_I could result from the interaction of two mobile C_I defects. We did not investigate this reaction here: on one hand the C_I defect concentration in typical experimental conditions is pretty low to make the event of C_I pairing quite unlikely; on the other side, the attraction basin of the C_I pair depends on the orientation of the C_I defects and requires the exploration of a wide parameter space. We leave this for further work and consider this process as an alternative way to form the C_IC_I complex.

D. Formation of the C_II defect

The last process we studied is the capture of a self-interstitial silicon by a carbon interstitial, as shown in Fig. 5 (top panel). The corresponding binding-energy plots are reported in Fig. 5 (middle and bottom panels).

We consider again two possibilities: I moves towards C_I along the upper or lower bond chain shown in Fig. 5 (top panel). Both paths have a first minimum corresponding to a precapture followed by small barrier before the final conversion into the stable complex. The structure of the complex after the capture process is shown in Fig. 4(d). On the left side we show the ideal silicon lattice around the defect while on the right side the defect is placed in the crystalline structure. We see that this defect consists of a Si-C split entirely contained in the interstitial cage of the silicon lattice. Each of the two defect atoms is threefold coordinated. The silicon lattice is nearly unaffected by the presence of this defect whose binding energy is a large 2.0 eV. This makes this complex a very stable one.

IV. DISCUSSION

In Fig. 6 we summarize all of the relevant carbon-silicon interactions involving up to two silicon self-interstitial defects; the zero of energy is defined for a crystalline system containing a reservoir of three C_S and two I noninteracting defects. Energy values correspond to *ab initio* results. The main message reported there is that the trapping of Si interstitials by C substitutional defects is in fact a multistep reaction, leading to the formation of a large variety of complexes.

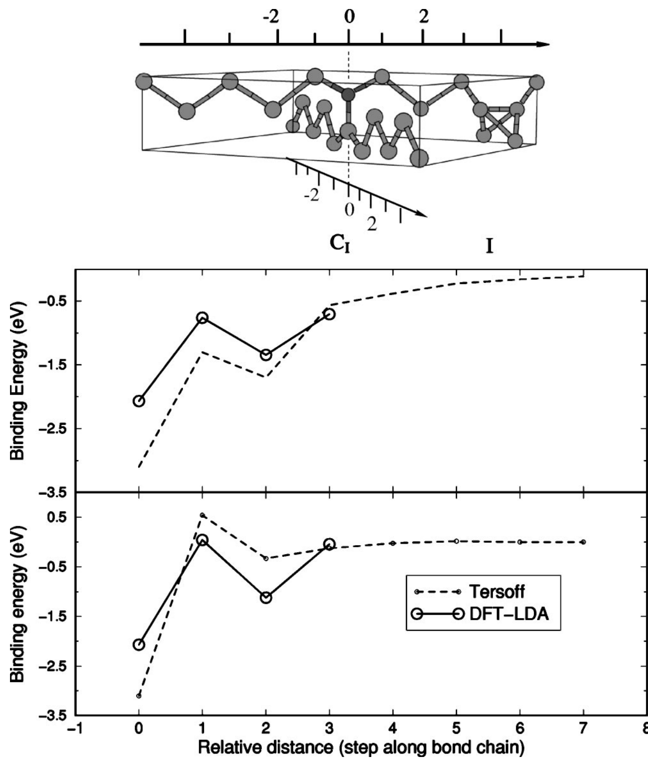

FIG. 5. Top panel: a carbon interstitial split C_I and a silicon interstitial I interacting along the $\langle 110\rangle$ reaction direction (upper chain) or along the $\langle \bar{1}10\rangle$ reaction direction (lower chain). Black: C; gray: Si. Bottom panels: Attraction basins between a C_I split and a I dumbbell along $\langle 110\rangle$ (middle panel) and $\langle \bar{1}10\rangle$ (bottom panel) directions.

The very first reaction (1) corresponds to the $C_S+I\rightarrow C_I$ capture; it turns out to be exothermic with a release of energy as large as 1.2 eV. Once the C_I defect is formed, it can hardly transform back into a C_S one since very few vacancies are typically available within an environment characterized by a supersaturation of Si interstitials. C_I is therefore the starting configuration for further evolution.

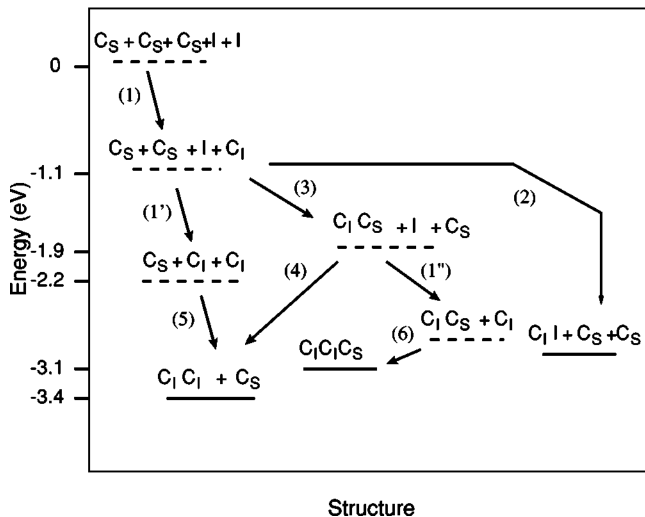

FIG. 6. Summary of all the mechanisms involving three carbon atoms C_S and two silicon self-interstitials I. The arrows define the possible reactions.

We indentified at least three possible pathways, hereafter labeled $(1')$–(3) (see Fig. 6): what really underlines the microstructural evolution is the actual relative abundance of different defect (either I or C_S) species. For instance, the $C_S+C_S+I+C_I$ system could evolve towards the $C_II+C_S+C_S$ configuration [reaction (2)] rather than into $C_S+C_I+C_I$ [reaction $(1')$] or $C_IC_S+I+C_S$ [reaction (3)] provided that an extremely high concentration of Si interstitials is found.

When the system follows the reaction (2) a very stable C_II defect is indeed formed; its unlikely that it transforms—upon additional capture of a C_S defect—into a C_IC_I complex since both C_II and C_S are immobile. On the other hand, C_II could trap more I's or C_I's, thus forming larger C_II_n or $(C_I)_nI$ complexes. This conclusion supports the experimental evidence according to which carbon implantation is very effective in reducing boron TED:[22] implanted carbon atoms—upon formation of C_II, C_II_n, or $(C_I)_nI$ complexes—may immobilize one or more Si interstitials and therefore effectively decrease their number. This in turn eventually reduces boron TED as clearly observed in experiments.[22,23]

A different scenario occurs when a comparatively higher concentration of C_S defects is observed. In this case, C_IC_S complexes are easily formed, as shown in Fig. 6 by reaction (3). Such a complex is, however, metastable (corresponding to a modest 0.8-eV energy release) and the reverse reaction can indeed occur at a typical annealing temperature (about 1000 K) where the configuration is dissociated. Before dissociation, however, C_IC_S can further trap another I defect following the reaction (4). This leads to the formation of the rather stable C_IC_I structure previously discussed. A possible alternative pathway towards the formation of C_IC_I is sketched by reactions $(1')+(5)$ which are estimated on the basis of the computed defect energetics (see previous section). Alternatively, C_IC_S could trap another C_I, as shown by reactions $(1'')+(6)$, forming a new $C_IC_IC_S$ complex. Its binding energy is, however, very low (about 0.2 eV).

On the basis of the above discussion, we can provide a rationale for the observed behavior of carbon diffusion and precipitation in $Si_{1-x}C_x$ layers.[12,16] Let us consider a C-doped silicon sample where an external source of Si interstitials is available and let us suppose that the relative occurrence of I's is much lower than the C_S's. The interaction among C_I's/I's and C_S's is accordingly rather infrequent so that most of the C_IC_S complexes dissociate without further interacting with other defects. In this condition, C_IC_S complexes do not firmly immobilize the C interstitials; rather they simply reduce the diffusivity of carbon by a sequence of "stop-and-go" events at the substitutional carbon centers.[14] This mechanism does not allow for the clustering of carbon. Accordingly, we suggest that C clustering is indeed possible only at higher I content. We further remark that the coalescence phenomenon requires at least the pairing of the C_IC_S with a second interstitial defect (I or C_I) before it could dissociate.

Overall the above picture nicely agrees with the experi-

mental findings of Mirabella *et al.* They studied a layer of silicon with a high concentration of substitutional carbon, corresponding to $x \sim 10^{-4}$. They found that in the presence of Si interstitials flux the carbon defects are efficiently immobilized by means of trapping events. This process proceeds until the formation of Si-C complexes. Conversely, in the same thermal conditions but with no Si interstitials flux, carbon atoms do not precipitate and diffuse away from the $Si_{1-x}C_x$ layer.

In conclusion, we suggest the existence of three possible regimes for carbon diffusion and aggregation defined by the actual Si interstitials content: (i) at low I content, C_I defects diffusion is mediated by capture-release processes; (ii) at high I content, the C_IC_S defect further interacts with silicon and carbon interstitials, giving rise to the coalescence process for carbon atoms; (iii) at very high I content, C_I is likely to interact directly with I's forming a remarkably stable C_II defect.

V. CONCLUSIONS

We have investigated the processes originating from the interaction of self-interstitial silicon atoms in C-doped crystalline silicon, using a combination of model-potential molecular-dynamics and first-principles calculations. We have found that besides the well-known C_IC_S carbon complex, other defects can form after the capture of up to two I by substitutional carbons. The simulations performed using model-potential MD, validated by first-principles calculations, show a variety of possible I and C_I capture reactions. All of the reactions investigated here are found to be exothermic: The corresponding capture events are therefore likely at the typical experimental annealing temperatures.

We finally discussed the influence of these defects on the diffusion and precipitation of carbon atoms in the presence of silicon self-interstitials. We characterized the formation process of the well-known C_IC_S defect which turned out to be just one among many other possible reactions leading to carbon immobilization. As the concentration of self-interstitials rises over the thermal equilibrium concentration, other Si-C trapping mechanisms begin to be effective; in particular, we have identified those leading to the formation of C_IC_I and C_II complexes. We believe that the inclusion of these additional reaction processes would be of great help in a more fundamental and predictive understanding of C-related silicon bulk processing.

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[1] P.A. Stolk, D.J. Eaglesham, H.-J. Gossmann, and J.M. Poate, Appl. Phys. Lett. **66**, 1370 (1995).

[2] E. Napolitani, A. Coati, D. De Salvador, A. Carnera, S. Mirabella, S. Scalese, and F. Priolo, Appl. Phys. Lett. **79**, 4145 (2001).

[3] P.A. Stolk, H.-J. Gossmann, D.J. Eaglesham, D.C Jacobson, C.S. Rafferty, G.H. Gilmer, M. Jaraiz, J.M. Poate, H.S. Luftman, and T.E. Haynes, J. Appl. Phys. **81**, 6031 (1997).

[4] P. Werner, H.-J. Gossmann, D.C. Jacobson, and U. Gösele, Appl. Phys. Lett. **73**, 2465 (1998).

[5] G.D. Watkins and K.L. Brower, Phys. Rev. Lett. **36**, 1329 (1976).

[6] R.B. Capaz, A. Dal Pino, Jr., and J.D. Joannopoulos, Phys. Rev. B **50**, 7439 (1994).

[7] L.W. Song, X.D. Zhan, B.W. Benson, and G.D. Watkins, Phys. Rev. Lett. **60**, 460 (1988).

[8] J. Tersoff, Phys. Rev. Lett. **64**, 1757 (1990).

[9] R.B. Capaz, A. Dal Pino, Jr., and J.D. Joannopoulos, Phys. Rev. B **58**, 9845 (1998).

[10] J. Zhu, Comput. Mater. Sci. **12**, 309 (1998).

[11] P. Leary, R. Jones, S. Öberg, and V.J.B. Torres, Phys. Rev. B **55**, 2188 (1997).

[12] S. Mirabella, A. Coati, D. De Salvador, E. Napolitani, A. Mattoni, G. Bisognin, M. Berti, A. Carnera, A.V. Drigo, S. Scalese, S. Pulvirenti, A. Terrasi, and F. Priolo, Phys. Rev. B **65**, 045209 (2002).

[13] J.L. Ngau, P.B. Griffin, and J.D. Plummer, J. Appl. Phys. **90**, 1768 (2001).

[14] R. Pinacho, M. Jaraiz, H.J. Gossmann, G.H. Gilmer, J.L. Benton, and P. Werner, in *Si Front-End Processing—Physics and Technology of Dopant-Defect Interactions II*, edited by A. Agarwal, L. Pelaz, H-H. Vuong, P. Packan, and M. Kase, Mater. Res. Soc. Symp. Proc. No. 610 (Materials Research Society, Pittsburgh, 2001).

[15] M.D. Johnson, M.-J. Caturla, and T. Diaz de la Rubia, J. Appl. Phys. **84**, 1963 (1998).

[16] H. Rücker, B. Heinemann, D. Bolze, R. Kurps, D. Krüger, G. Lippert, and H.J. Osten, Appl. Phys. Lett. **74**, 3377 (1999).

[17] J. Tersoff, Phys. Rev. B **39**, 5566 (1989).

[18] G. Kresse and J. Hafner, Phys. Rev. B **47**, R558 (1993); G. Kresse, Ph.D. thesis, Technische Universität Wien, 1993; G. Kresse and J. Furthmüller, Comput. Mater. Sci. **6**, 15-50 (1996); Phys. Rev. B **54**, 11 169 (1996).

[19] D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990).

[20] M. Tang, L. Colombo, J. Zhu, and T. Diaz de la Rubia, Phys. Rev. B **55**, 14 279 (1997).

[21] C.-L. Liu, W. Windl, L. Borucki, S. Lu, and X.-Y. Liu, Appl. Phys. Lett. **80**, 52 (2002).

[22] N.E.B. Cowern, A. Cacciato, J.S. Custer, F.W. Saris, and W. Vandervorst, Appl. Phys. Lett. **68**, 1150 (1996).

[23] U. Gösele, P. Laveant, R. Scholz, N. Engler, and P. Werner, in *Si Front-End Processing-Physics and Technology of Dopant-Defect Interactions II*, edited by A. Agarwal, L. Pelaz, H-H. Vuong, P. Packan, and M. Kase, Mater. Res. Soc. Symp. Proc. No. 610 (Materials Research Society, Pittsburgh, 2000).