Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physica B 340–342 (2003) 729–733
PHYSICA B
www.elsevier.com/locate/physb

Electrical signature for configurational bistability of self-interstitial clusters in ion-damaged silicon

P.K. Giri*

Department of Physics, Indian Institute of Technology, Guwahati 781039, Assam, India

Abstract

Self-interstitial clusters introduced by high-energy Ar ion implantation in silicon are studied by capacitance transient spectroscopic techniques. Trapping kinetics studies at low temperature over a wide range of trap-filling time reveal the presence of three trap levels, two of which are interrelated. A detailed analysis of the trap occupancy features using numerical simulation show that the two interrelated traps are two configurations of the same defect. From model simulation, it is also shown that exact occupancy features observed experimentally could be fitted by assuming the metastable defect to be a negative-U (Hubbard correlation energy) center.

Keywords: Metastable defects; Interstitial clusters; DLTS; Ion irradiation

1. Introduction

Under suitable thermodynamic conditions, interstitial and vacancy clusters can be produced by ion implantation in semiconductors. At present, self-interstitial (I) clusters are extensively studied in silicon due to their interesting electronic, optical and vibration properties [1,2]. However, experimentally very little is known about self-interstitial clusters due to their inaccessibility to conventional experimental tools. The electrical signature of self-interstitial clusters and their thermal stability has been obtained [3,4] using deep level transient spectroscopy (DLTS). Optical studies have shown that some form of I-cluster is responsible for the well-known W-band photoluminescence (PL) in silicon [5]. Recently, theoretical studies have shown that I-clusters are most likely to be responsible for dislocation related D-band photoluminescence and, consequently, it has triggered a large interest in the study of small I-clusters [6] in silicon.

Molecular dynamics studies on self-interstitial aggregates in Si show that the potential energy surfaces for aggregates of three or more I's have several local minima, leading to a range of metastable configurations [7]. It has been predicted that I_3-clusters in Si are most likely to exhibit metastability. However, no experimental evidence is available yet in the literature in support of this proposition.

In this article, we report on the metastability of I-clusters created by heavy ion damage in silicon and studied by isothermal capacitance transient spectroscopic technique. Through trapping kinetics studies at a fixed temperature, we show that the small I-clusters exhibit metastability upon

*Fax: +91-361-2690762.
E-mail address: giri@iitg.ernet.in (P.K. Giri).

0921-4526/$ - see front matter © 2003 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2003.09.109

capture of carriers at the defect. Model simulation predicts that configurational bistability of the I-cluster is responsible for the observed trap occupancy features.

2. Experimental details

Self-interstitial clusters were created in phosphorus doped n-type epitaxial Si wafers by irradiating the wafers with 1.45 MeV Ar^+ ions at fluences of 5×10^{13} and $1\times10^{14}\,cm^{-2}$. Ar^+ ion was chosen for implantation, as it is known to be a source of self-interstitials in silicon. For wire bonding to the Schottky contacts, all the samples were subjected to 70°C oven annealing for 30 min. Some samples were post-annealed at 160°C for various durations for studying the stability of the defects. The capacitance measurements were done using a Boonton capacitance meter operated at 1 MHz. DLTS was used for survey of the defects and time analyzed transient spectroscopy (TATS) was used for studying trapping kinetics at the defect clusters. As the defect density is very large in these samples, the measurement was performed in the constant capacitance mode using a feedback circuit. Traps were filled with carriers by collapsing the depletion layer (with zero bias) for a pre-selected time.

3. Results and discussion

Fig. 1 shows a typical set of DLTS spectra for Si implanted with 1×10^{14} Ar^+ ions/cm^2 and annealed at 160°C for 30 min or 3 h. Each spectrum is dominated by two peaks, P1 and P2. Peak P1 is attributed to the well-known divacancy trap with energy $E_C-0.42$ eV. Peak P2 has been attributed to the formation of self-interstitial clusters in Si. The intensity and position of peak P2 changes with annealing conditions as shown in the figure. Processing induced change in energy level ($E_C-0.49$ eV to $E_C-0.56$ eV) and energy broadening (up to 25 meV) of the trap hint to a change in the structure of the defect. This is considered as an important hint to anticipate metastability in such defects. Though definite identification of the defect

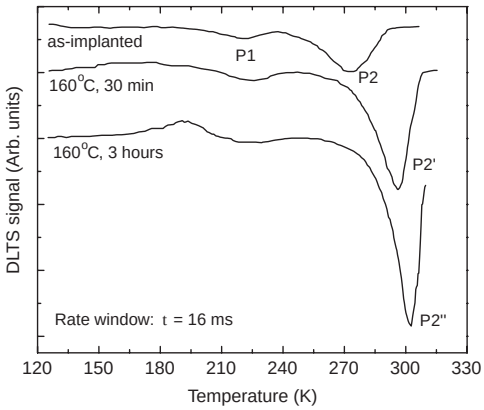

Fig. 1. A set of DLTS spectra showing the evolution of peak P2 for: (1) as-implanted Si; (2) 160°C, 30 min post-annealed; (3) 160°C, 3 h post-annealed.

is unknown at present, in accordance with the literature reports, peak P2 is likely to arise from tri-interstitial (I_3) or tetra-interstitial (I_4) clusters in silicon [2,8].

To study trapping kinetics at these defects, TATS spectra were recorded for various filling time at a fixed temperature. In Fig. 2, a set of TATS spectra is shown for high fluence implanted sample for progressively increasing filling times over five orders in magnitude. It was found that peak P1 is very broad and peak shape changes with filling time duration. In Fig. 2, peak P1 is fitted (dotted lines) to two emitting centers (P1A and P1B) assuming a Gaussian broadening of 10 meV in activation energy and peak P2 is fitted with a Gaussian broadening of 25 meV in activation energy, which is believed to result from the strain in the clusters. The peak intensities obtained from such an analysis have been plotted as a function of the logarithm of filling time in Fig. 3. Peak P1A initially increases, going through a maximum at a filling time approximately equal to its emission time constant (τ_e). An increase in intensity of peak P2 occurs when peak P1A starts to decrease. Peak P1B also goes through a maximum for longer filling times. These general features are common to samples irradiated with two different doses. Clearly, this is a case of coupled carrier kinetics with multiple traps. Note that the apparent shift of peaks P1A and P1B in

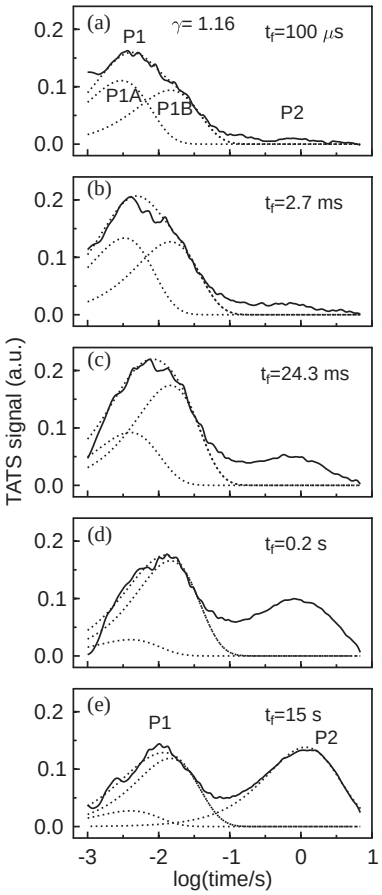

Fig. 2. CC-TATS spectra of as-implanted Si at 217.6 K for different filling time, showing progressive change in occupancy. Peak P1 is fitted (dotted line) with two different centers P1A and P1B. Peak P2 is fitted with a Gaussian broadened energy level.

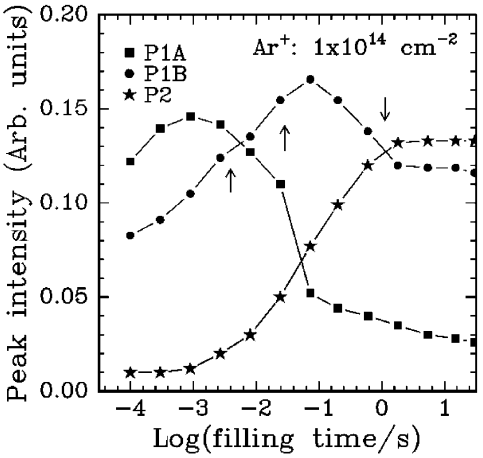

Fig. 3. Occupancy feature of peak P1A, P1B and P2 as a function of filling time. Arrows indicate the measured time constants (τ) for the corresponding traps.

Fig. 2 is not due to any change in energy of the defect in question, but rather to a relative occupancy change of the constituent peaks.

It is observed from the trap occupancy feature that the shallow states lose charges to deeper ones, when filling times are larger than their characteristic emission time (respective τ_e's shown with arrow in Fig. 3). This suggests a redistribution of charges through multiple trapping. However, model simulation assuming three independent traps (shown in Fig. 4(a)) shows that simple charge redistribution among independent states cannot account for the observed occupancy features. We have performed a detailed simulation for occupancy features using various coupling mechanisms, which could be broadly classified as serial (hierarchical) and parallel process of charge relaxation. A detailed discussion about these models has been presented in Ref [9]. In view of the simulation results, to explain the occupancy features observed in Fig. 3, we need to assume that peaks P1A and P2 are two different configurations of the same defect. The rate equations are expressed as:

$$\dot{n}_1 = -e_1 n_1 + c_1 n((N_{T1} + N_{T3})/N_T - n_1 - n_3), \quad (1)$$

$$\dot{n}_2 = -e_2 n_2 + c_2 n(N_{T2}/N_T - n_2), \quad (2)$$

$$\dot{n}_3 = -e_3 n_3 + c_3 n((N_{T1} + N_{T3})/N_T - n_1 - n_3) \quad (3)$$

with the constraint on number of electrons

$$n = 1 - n_1 - n_2 - n_3. \quad (4)$$

In the above equations, n_1, n_2, n_3 are the normalized (with respect to N_T, the total trap concentration) trap concentrations, e_1, e_2, e_3 are respective emission rates, c_1 c_2, c_3 are the respective capture rates for three trap levels, and n is the free electron concentration (normalized). Fig. 4(b) shows the occupancy features in such a case. Here, we have assumed that $N_{T1} + N_{T3} = 0.5N_T$ and $N_{T2} = 0.5N_T$. However, a more accurate description of the

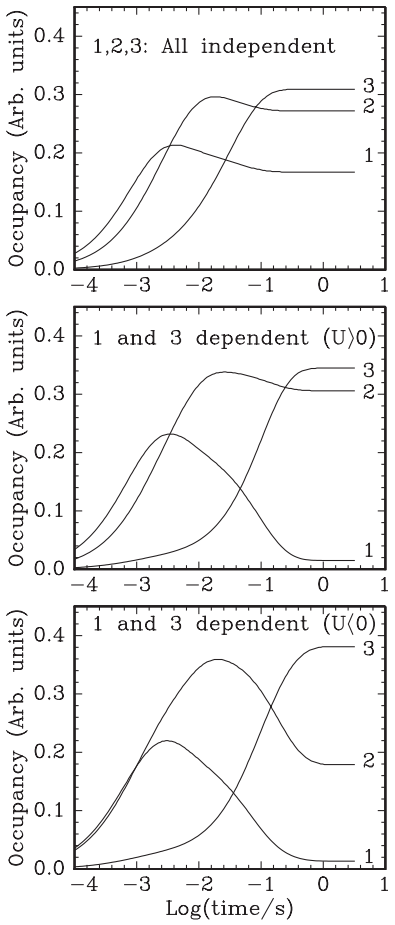

Fig. 4. Simulated trap-occupancy features assuming: (a) three independent traps; (b) 1 and 3 are two configurations of the same defect with $U>0$; (c) two configurations with $U<0$. Simulation parameters: $c_1=1000$, $c_2=400$, $c_3=80$, $e_1=200$, $e_2=40$, $e_3=0.7$ (all in s^{-1} units).

coupling among these three defects could be obtained by assuming the metastable defect to be a negative-U (Hubbard correlation energy) center. With the negative-U condition, Eq. (4) will be modified as

$$n = 1 - 2n_1 - n_2 - 2n_3. \quad (5)$$

Note that in the above equation, the prefactor 2 for n_1 and n_3 accounts for the doubly occupied negative-U states of the defects. The simulation results shown in Fig. 4(c) matches very well with the experimental features, particularly relating to the decrease of occupancy of trap P2 for longer filling times. Thus, it is understood from simulation that the configurationally bistable defect is a negative U center. The negative U could arise due to a strong coupling of the defect to the lattice relaxation and vibration. We anticipate small interstitial clusters to behave as negative-U centers possibly along with large lattice relaxation due to the involvement of several lattice sites. I_3 cluster in Si is predicted to have a metastable configuration as the defect occupies BC sites and the I's can exchange sites with each other [6]. Hence, the observed defect P2 may have direct correlation with the proposed metastable I_3^b structure. PL studies on ion implanted Si usually show W-band that has been related to I_3-clusters and the density of these defects grows with annealing up to a temperature of $\sim$250°C [5]. Our DLTS studies also show that the cluster related peak grows with low-temperature annealing (160°C) and thus has direct correlation with the PL behavior of the I_3-cluster in Si. Hence, it is believed that in our as-implanted samples I_3-cluster is the most probable candidate possessing the observed metastability.

4. Conclusions

We have provided electrical signature for configurational bistability of self-interstitial clusters in ion-damaged silicon through trapping kinetics studies. Studies at low temperature show a parallel relaxation of charge through multiple traps via coupled dynamics. Using model simulations, a detailed analysis of the trap occupancy features show that the I-cluster exists in two different configurations and the shallower state is an unstable configuration, observable for short filling time. From simulation result, it is also predicted that the observed metastable defect is a negative-U center.

References

[1] N. Arai, S. Takeda, M. Kohyama, Phys. Rev. Lett. 78 (1997) 4265;
M. Kohyama, S. Takeda, Phys. Rev. B 60 (1999) 8075.

[2] B.J. Coomer, P.J. Goss, R. Jones, S. Oberg, P.R. Briddon, J. Phys.: Condens. Matter 13 (2001) L1.
[3] S. Libertino, S. Coffa, J.L. Benton, Phys. Rev. B 63 (2001) 195206.
[4] P.K. Giri, Defects Diffus. Forum 210–212 (2002) 1.
[5] P.K. Giri, S. Coffa, E. Rimini, Appl. Phys. Lett. 78 (2001) 291.
[6] S.K. Estreicher, M. Gharaibeh, P.A. Fedders, P. Ordejon, Phys. Rev. Lett. 86 (2001) 1247.
[7] M. Gharaibeh, S.K. Estreicher, P.A. Fedders, Physica B 273–274 (1999) 532.
[8] B.J. Coomer, P.J. Goss, R. Jones, S. Oberg, P.R. Briddon, Physica B 273–274 (1999) 505.
[9] P.K. Giri, Y.N. Mohapatra, Phys. Rev. B 62 (2000) 2496.