Isochronal annealing studies of carbon-related defects in irradiated Si

C.A. Londos*, M.S. Potsidi, G.D. Antonaras, A. Andrianakis

University of Athens, Solid State Physics Section, Panepistimiopolis, Zografos, Athens 157 84, Greece

Abstract

We report infrared spectroscopy studies of defects in neutron-irradiated, carbon-doped, Cz-grown silicon. At room temperature irradiations, among the main defects formed are the CiCs and CiOi complexes. A peak in the spectra at 544 cm\(^{-1}\) was found to be the contribution of two bands at 543.5 and 545.5 cm\(^{-1}\). From the corresponding annealing behavior of these bands, the 543.5 cm\(^{-1}\) band was correlated with the CiCs defect although the 544.5 cm\(^{-1}\) disappearance is not accompanied by the emergence of any signal. The CiCs and the CiCs contribution of two bands at 543.5 and 545.5 cm\(^{-1}\) have been correlated with the CiCs defect although the 544.5 cm\(^{-1}\) band with the CiOi defect. At high-irradiation doses, complexes as the Ci(Si)\(_1\) (953, 960 cm\(^{-1}\)), CiO(Si)\(_1\) (934, 1018 cm\(^{-1}\)), CiCs(Si)\(_1\) (987, 993 cm\(^{-1}\)) and CiCs (527 cm\(^{-1}\)) form. Isochronal anneals performed in order to study the thermal evolution of these centers, showed that the Ci(Si)\(_1\) and CiO(Si)\(_1\) begin to decay in the spectra around 150 °C. Their disappearance is not accompanied by the emergence of any signal. The CiCs and the CiCs(Si)\(_1\) centers begin to decay around ~250 °C. Their disappearance is accompanied by the emergence of two pairs of bands at (918, 1006 cm\(^{-1}\)) and (945, 964 cm\(^{-1}\)), respectively. The origin of the centers, giving rise to these bands is discussed.

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1. Introduction

Carbon is, besides oxygen, the most important impurity in Si. It has been studied intensively during the last 50 years. However, in spite of the very large amount of work that has been done so far, some aspects of its behavior, especially those concerning the reaction processes that carbon participates in, are not known in detail. Upon irradiation of carbon-rich Cz-grown Si, carbon-substitutional atoms (Ci) are ejected [1] at interstitial sites (Ci), according to the Watkins-replacement mechanism (Ci + Si\(_i\) → Ci). Ci is very mobile at room temperature and it readily reacts [2] with Si\(_i\) and O\(_i\) defects forming the CiCs and CiOi pairs, respectively. Most of the primary defects produced by the irradiation tend to annihilate between themselves (V + Si\(_i\) → O), although some of them are captured by impurities present in the material (V + O\(_i\) → VO, Si\(_i\) + C\(_i\) → C\(_i\), etc.) and some other pair with each other (V + V → V\(_2\), Si\(_i\) + Si\(_i\) → (Si\(_i\)−Si\(_i\))). Defect reaction modeling foresees and experiments verify [3–5] that a percentage of the Si\(_i\)'s is also captured by centers formed during the irradiation. Thus, the Ci, the CiCs and CiOi defects act as nucleation sites for the Si\(_i\)'s and at high radiation doses, complexes as the Ci(Si)\(_1\), the CiO(Si)\(_1\) and the CiCs(Si)\(_1\) form, as well. A pair of local vibrational mode (LVM) bands at (953, 966 cm\(^{-1}\)) has been correlated [2] with the Ci(Si)\(_1\), another pair at (940, 1024 cm\(^{-1}\)) has been correlated [2] with the CiO(Si)\(_1\) complex and another one at (987, 993 cm\(^{-1}\)) has been correlated [6] with the CiCs (Si)\(_1\) complex. On the other hand, vacancies are also trapped by the CiCs complexes [7] leading to the formation of the CiCs defect (527.4, 748.7 cm\(^{-1}\)), through the reaction CiCs + V → CiCs.

In neutron-irradiated Si, due to the spatial separation [8] of the produced vacancies and self-interstitials, complexes related to these defects form in larger concentrations. Therefore, weak signals in the spectra related to such complexes are expected to be detected more easily, facilitating their study. The purpose of this work is to study the production and evolution with temperature of the Ci(Si)\(_1\), CiCs(Si)\(_1\), CiO(Si)\(_1\) and CiCs defects. It is a

*Corresponding author. Tel./fax: +30 210 7276726.
E-mail address: hlontos@phys.uoa.gr (C.A. Londos).

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continuation of a previous work [6], aiming in particular at throwing new light on carbon-related defects and processes, where aggregations of primary defects are involved.

2. Experimental details

Prepolished Si samples of 2 mm thickness with initial oxygen and carbon concentrations $[O_i]_o = 7.2 \times 10^{17}$ cm$^{-3}$ and $[C_o]_o = 1.5 \times 10^{17}$ cm$^{-3}$, respectively, were irradiated with 5 MeV fast neutrons at a fluence of $\sim 1 \times 10^{17}$ n/cm$^2$. The samples were wrapped in Cd foils to eliminate thermal neutrons and put inside sealed quartz boxes to avoid water contamination. After the irradiations, 20 min isochronal anneals of $\sim 10$°C steps, in open furnaces were performed. After each annealing stage, infrared spectroscopy measurements were carried out, at room temperature, with a Jasco-IR 700 double beam dispersive spectrometer.

3. Experimental results and discussion

Fig. 1 shows a section of the absorption spectrum of our Si samples immediately after the irradiation. By using Lorentzian profiles (Fig. 2a) it is found that the band at 544 cm$^{-1}$ is the overlap of two contributing bands at 543.5 and 545.5 cm$^{-1}$. Figs. 2(b) and (c) exhibit the thermal evolution of the latter bands. Previously IR studies [9], in electron-irradiated Si, have detected the formation of the $C_iC_s$ center and six bands at 540.4, 543.3, 579.8, 640.6, 730.4 and 842 cm$^{-1}$ have been attributed to the B configuration of the defect, corresponding to its neutral charge state, in which the center is expected to be in irradiated material. These bands are seen only at liquid He temperatures. They are very weak, and this fact along with strong unharmonic effects [9,10] prevents their detection at room temperature. The bands are stable up to $\sim 250$°C. It has also been reported [11,12] that a band at $\sim 540$ cm$^{-1}$, detected in electron-irradiated material at liquid He temperatures, being stable up to $\sim 300$°C is related to the $C_iC_s$ center. Thus, in our case, where both the $C_iC_s$ and $C_iO_i$ defects are expected to form and be stronger due to the neutron irradiation, we can reasonably assume that they contribute to the same broad peak making their signal

![Fig. 1. Section of absorption spectrum of neutron-irradiated, carbon-doped, Cz-grown Si.](image)

![Fig. 2. (a) Lorentzian profiles of the 544 cm$^{-1}$ IR band, (b) the thermal evolution of the 543.5 and the (918,1006 cm$^{-1}$) pair of bands, (c) the thermal evolution of the 545.5 cm$^{-1}$ band.](image)
detectable at room temperature. In this sense, based on their annealing behavior (Figs. 2(b) and (c)) we correlate the bands at 543.5 and 545.5 cm\(^{-1}\) with the C\(_1\)C\(_4\) and C\(_1\)O\(_1\) defects, correspondingly. We note at this point that the decay of the 543.5 cm\(^{-1}\) band is accompanied in the spectra (Fig. 2(b)) by the emergence of two bands at 918 and 1006 cm\(^{-1}\) (Fig. 3).

As we mentioned in the Introduction, the Si\(_1\)'s tend to aggregate on carbon-related complexes. Fig. 4(a) shows a section of the absorption spectrum received immediately after the irradiation. The pairs of bands at (953, 960 cm\(^{-1}\)), (934, 1018 cm\(^{-1}\)) and (987, 993 cm\(^{-1}\)) have been previously attributed \cite{2,6} to the C\(_1\)(Si\(_1\)), C\(_1\)O\(_1\)(Si\(_1\)) and C\(_4\)C\(_4\)(Si\(_1\)) complexes, respectively. Figs. 4(b) and (c) show the evolution with temperature of the C\(_1\)(Si\(_1\)) and C\(_1\)O\(_1\)(Si\(_1\)) complexes, respectively.

The decay of the corresponding peaks is not accompanied by the emergence of other peaks in the spectra. Further on, Fig. 5(a) shows the thermal evolution of the (987, 993 cm\(^{-1}\)) pair of bands the decay of which is accompanied by the emergence in the spectra of two bands at 945 and 964 cm\(^{-1}\) (Fig. 5(b)). Photoluminescence studies \cite{13,14} have reported that the destruction of the 969 meV PL line of the C\(_4\)C\(_4\) defect (G-line) is partly connected with the growth of lines at 951, 953, 954 and 957 meV which have been attributed to G-centers perturbed by nearby self-interstitials. Additional PL lines have been reported \cite{16} to arise upon the destruction of the G-line of the C\(_4\)C\(_4\) defect. Moreover, a line at 949.9 meV, the so-called F-line, has been suggested \cite{17} to arise from a C\(_3\)O defect formed when a mobile C\(_4\)C\(_4\) defect is captured by a C\(_3\)O defect. We suggest that our pairs of LVM bands at (918, 1006 cm\(^{-1}\)) (Fig. 2(b)) and (945, 964 cm\(^{-1}\)) (Fig. 5(a)), may arise from the same centers that give rise to the above PL lines. Our suggestion is based mainly on the similarities in the emergence of the bands from the IR and PL studies and at this stage, any positive identification by assigning certain IR bands to certain structure cannot be made.

Vacancies also aggregate on carbon-related defects produced by the irradiation, leading to the formation of larger complexes. Such a complex is the C\(_3\)C\(_4\) structure.

Fig. 3. Section of the absorption spectrum showing the 918 and 1006 cm\(^{-1}\) bands.
which forms through the reaction \( \text{C}_4\text{C}_s + V \rightarrow \text{C}_4\text{C}_s \). In its neutral charge state, the defect gives rise to an IR band at 527 cm\(^{-1}\). In our neutron-irradiated samples, a band at 527 cm\(^{-1}\) was detected at room temperature (Fig. 1), tentatively attributed to the \( \text{C}_4\text{C}_s \) defect. Its evolution with temperature is given in Fig. 6.

4. Summary

We have investigated carbon-related complexes in neutron-irradiated Si, by means of IR spectroscopy. A broad band at 544 cm\(^{-1}\) was found to be the convolution of two bands at 543.5 and 545.5 cm\(^{-1}\). Based on their thermal stability, we attributed these bands to the \( \text{C}_4\text{C}_s \) and the \( \text{C}_4\text{O}_1 \) defects, correspondingly. The evolutions with temperature of the \( \text{C}_4\text{O}_1 \) (953, 960 cm\(^{-1}\)), \( \text{C}_4\text{O}_1 \) (934, 1018 cm\(^{-1}\)) and \( \text{C}_4\text{C}_s \) (987, 993 cm\(^{-1}\)) complexes were studied. Further on, a band at 527 cm\(^{-1}\) was tentatively attributed to the \( \text{C}_4\text{C}_s \) center.

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