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Isochronal annealing studies of carbon-related defects in irradiated Si

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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 C_iC_s and C_iO_i 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 C_iC_s defect although the 544.5 cm^{-1} band with the C_iO_i defect. At high-irradiation doses, complexes as the $C_i(Si_I)$ (953, 960 cm^{-1}), $C_iO_i(Si_I)$ (934, 1018 cm^{-1}), $C_iC_s(Si_I)$ (987, 993 cm^{-1}) and C_sC_s (527 cm^{-1}) form. Isochronal anneals performed in order to study the thermal evolution of these centers, showed that the $C_i(Si_I)$ and $C_iO_i(Si_I)$ begin to decay in the spectra around 150 °C. Their disappearance is not accompanied by the emergence of any signal. The C_iC_s and the $C_iC_s(Si_I)$ 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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Keywords: Silicon; Carbon impurity; Irradiation

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 (C_s) are ejected [1] at interstitial sites (C_i), according to the Watkins-replacement mechanism ($C_s + Si_I \rightarrow C_i$). C_i is very mobile at room temperature and it readily reacts [2] with C_s and O_i defects forming the C_iC_s and C_iO_i pairs, respectively. Most of the primary defects produced by the irradiation tend to annihilate between themselves ($V + Si_I \rightarrow Ø$), although some of them are captured by impurities present in the material ($V + O_i \rightarrow VO, Si_I + C_s \rightarrow C_i$, etc.) and some other pair with each other ($V + V \rightarrow V_2$, $Si_I + Si_I \rightarrow (Si_I - Si_I)$). 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 C_i, the C_iC_s and C_iO_i defects act as neucleation sites for the Si_I's and at high radiation doses, complexes as the $C_i(Si_I)$, the $C_iO_i(Si_I)$ and the $C_iC_s(Si_I)$ form, as well. A pair of local vibrational mode (LVM) bands at (953, 966 cm^{-1}) has been correlated [2] with the $C_i(Si_I)$, another pair at (940, 1024 cm^{-1}) has been correlated [2] with the $C_iO_i(Si_I)$ complex and another one at (987, 993 cm^{-1}) has been correlated [6] with the C_iC_s (Si_I) complex. On the other hand, vacancies are also trapped by the C_iC_s complexes [7] leading to the formation of the C_sC_s defect (527.4, 748.7 cm^{-1}), through the reaction $C_iC_s + V \rightarrow C_sC_s$.

In neutron-irradiated S_i, 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 $C_i(Si_I)$, $C_iC_s(Si_I)$, $C_iO_i(Si_I)$ and C_iC_s defects. It is a

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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 $[C_s]_o = 1.5 \times 10^{17}\,cm^{-3}$, 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 $\sim 10\,^{\circ}C$ 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 later 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 $842.4\,cm^{-1}$ 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 $\sim 250\,^{\circ}C$. It has also been reported [11,12] that a band at $\sim 540\,cm^{-1}$, detected in electron-irradiated material at liquid He

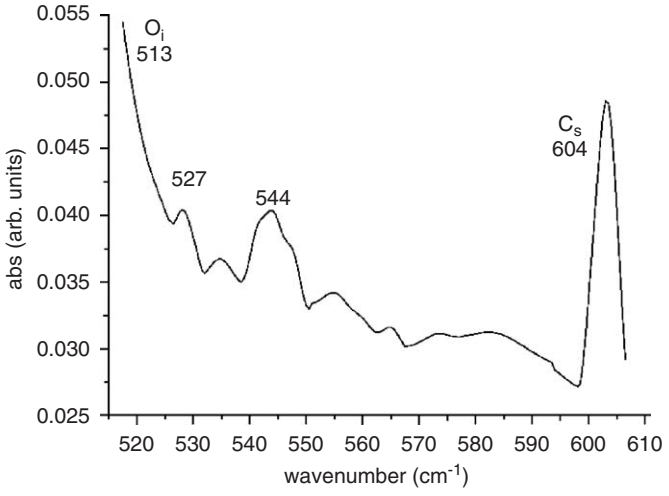

Fig. 1. Section of absorption spectrum of neutron-irradiated, carbon-doped, Cz-grown Si.

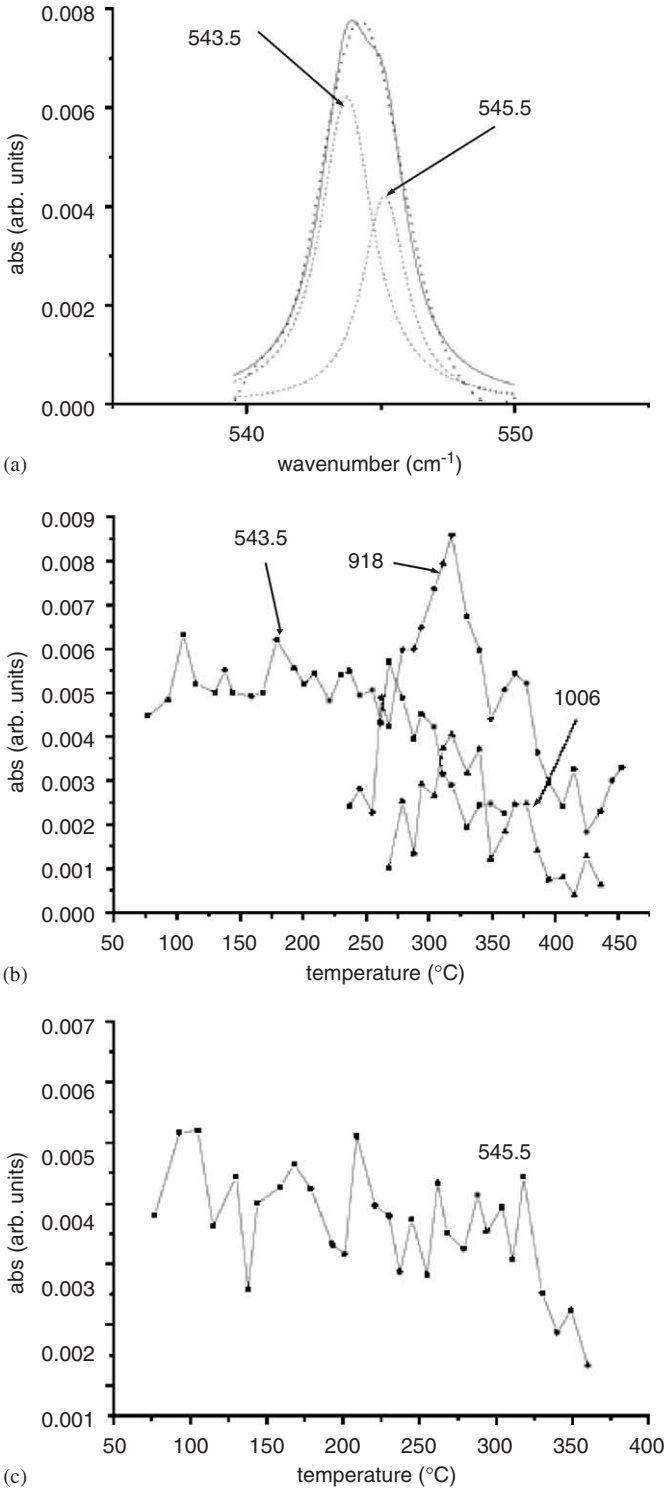

Fig. 2. (a) Lorentzian profiles of the $544\,cm^{-1}$ IR band, (b) the thermal evolution of the 543.5 and the $(918, 1006\,cm^{-1})$ pair of bands, (c) the thermal evolution of the $545.5\,cm^{-1}$ band.

temperatures, being stable up to $\sim 300\,^{\circ}C$ is related to the C_iO_i 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

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_iC_s and C_iO_i 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_I'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 [2,6] to the $C_i(Si_I)$, $C_iO_i(Si_I)$ and $C_iC_s(Si_I)$ complexes, respectively. Figs. 4(b) and (c) show the evolution with temperature of the $C_i(Si_I)$ and $C_iO_i(Si_I)$ 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 [13,14] have reported that the destruction of the 969 meV PL line of the C_iC_s 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 [16] to arise upon the destruction of the G-line of the C_iC_s defect. Moreover, a line at 949.9 meV, the so-called F-line, has been suggested [17] to arise from a C_3O defect formed when a mobile C_iC_s defect is captured by a C_iO_i 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.

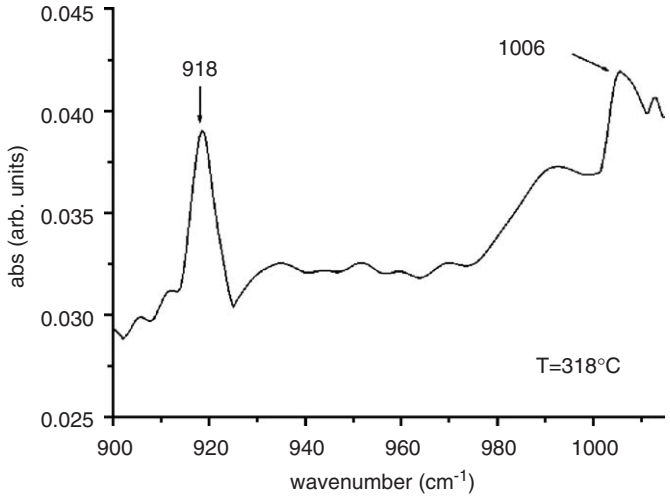

Fig. 3. Section of the absorption spectrum showing the 918 and 1006 cm^{-1} bands.

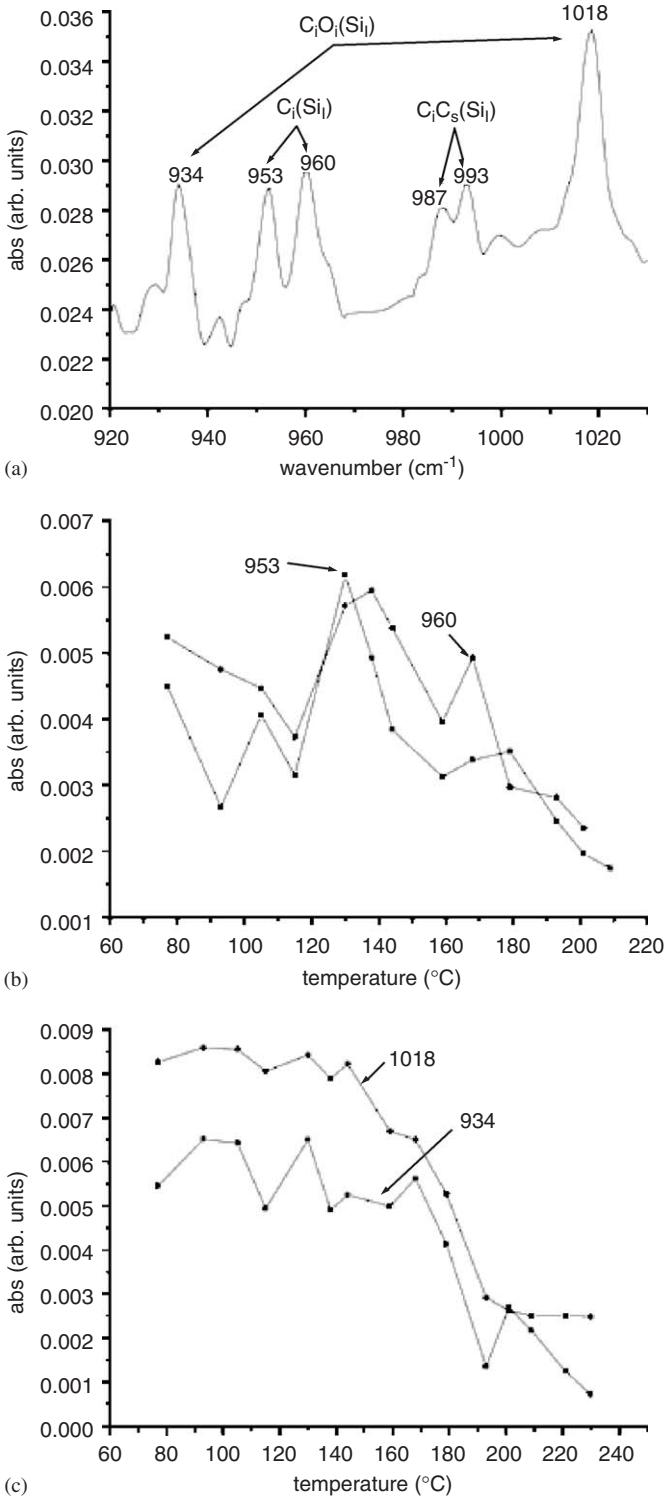

Fig. 4. (a) Section of absorption spectrum of neutron-irradiated, carbon-doped, Cz-grown Si taken immediately after room temperature irradiation, (b) the thermal evolution of the $(953, 960\,cm^{-1})$ bands of the $C_i(Si_I)$ defect, (c) the thermal evolution of the $(934, 1018\,cm^{-1})$ bands of the $C_iO_i(Si_I)$ defect.

Vacancies also aggregate on carbon-related defects produced by the irradiation, leading to the formation of larger complexes. Such a complex is the C_sC_s structure

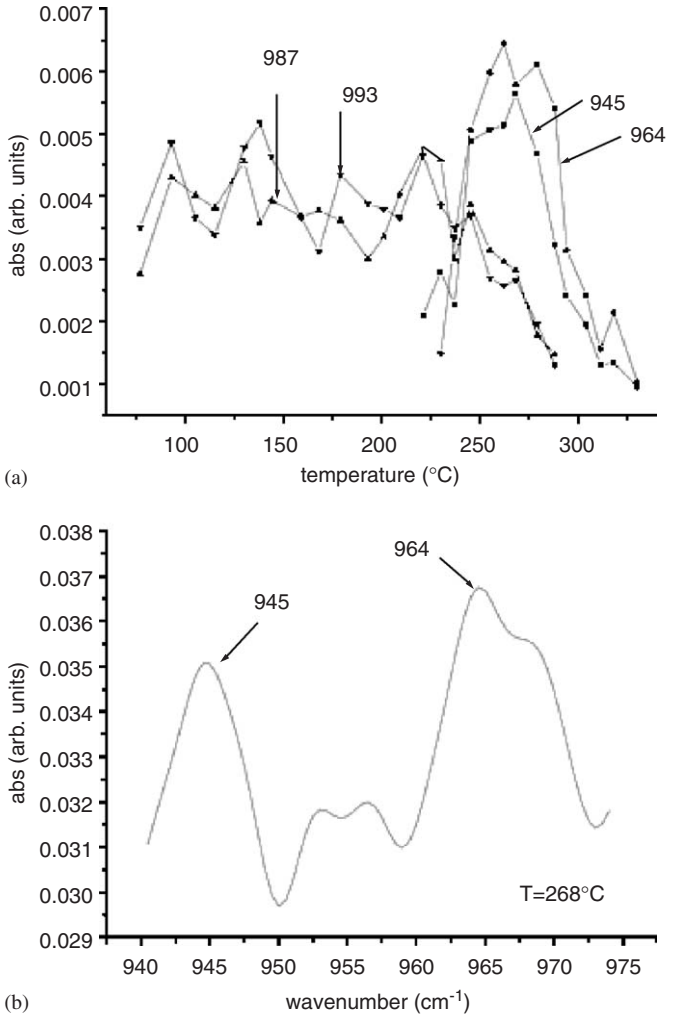

Fig. 5. (a) The thermal evolution of the (945 and 964 cm^{-1}) pair of bands grown in the spectra when the (987 and 993 cm^{-1}) pair of bands of the $C_iC_s(Si_I)$ defect anneals out, (b) section of the absorption spectrum showing the (945 and 964 cm^{-1}) pair of bands.

[7,15] which forms through the reaction $C_iC_s + V \rightarrow C_sC_s$. In its neutral charge state the defect gives rise to an IR band at 527.4 cm^{-1}. In our neutron-irradiated samples, a band at 527 cm^{-1}, detected at room temperature (Fig. 1), is tentatively attributed to the C_sC_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 C_iC_s and the C_iO_i defects, correspondingly. The evolutions with temperature of the $C_i(Si_I)$ (953, 960 cm^{-1}), $C_iO_i(Si_I)$ (934, 1018 cm^{-1}) and $C_iC_s(Si_I)$ (987, 993 cm^{-1}) complexes were studied. Further on, a band at 527 cm^{-1} was tentatively attributed to the C_sC_s center.

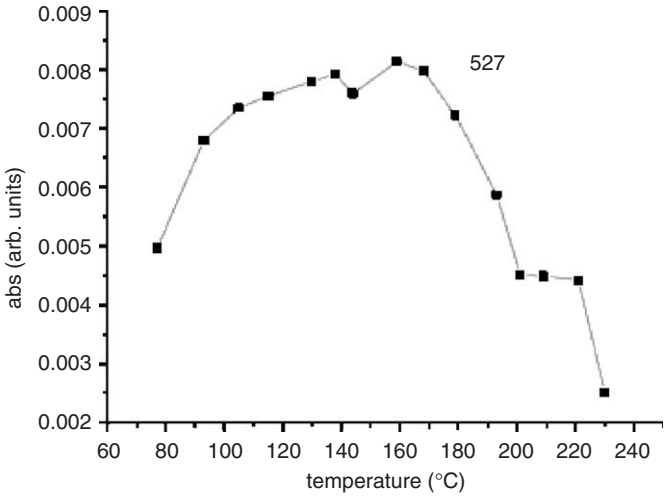

Fig. 6. The thermal evolution of the 527 cm^{-1} band.

Acknowledgments

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