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A spectroscopical study of the $C_iO_i(Si_i)$ absorption bands upon isothermal annealing in irradiated silicon at liquid helium temperatures (L.H.T.)

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The vast majority of modern electronic devices, is made by semiconducting materials such as crystalline Si. The wide-range of its applications makes it one of the most important semiconducting materials used in electronics industry and technology in general. The properties and behavior of silicon under varying conditions are studied ceaselessly the last 50 years in order to optimize the performance of devices based on this. Lattice defects created either by design or by different processes, influence the thermal, electrical, optical and other properties of Si. The most common method to induce defects in Czochralski Si (Cz-Si) controllably, is to irradiate it with electrons. The immediate products of the irradiation are vacancies (V) and self-interstitial atoms (Si_i) which react with other impurities to product complex defects. Carbon and oxygen are the main unintentionally added impurities in Si during growth. During irradiation or processing give rise to electrically active complex defects. Upon annealing oxygen acts as a trap [1] for carbon atoms to form the C_iO_i defect, which can trap [2] Si_i atoms to form the $C_iO_i(Si_i)$. This defect gives rise two main bands located at low temperatures at about 940 and 1024 cm^{-1} [3].

The aim of this work is to study via Infrared Spectroscopy, the thermal evolution of the $C_iO_i(Si_i)$ defect by measurements at liquid helium temperature (LHT). To this goal, a group of Cz-Si samples ($[O_i]_0=6.2 \times 10^{17} cm^{-3}$, $[C_i]_0=1.2 \times 10^{17} cm^{-3}$) was irradiated with 2 MeV electrons at a dose of $5 \times 10^{17} e^-/cm^2$, at a temperature $\sim 90^\circ C$. After irradiation, the corresponding values of oxygen and carbon concentration were 5.2×10^{17} and $0.62 \times 10^{17} cm^{-3}$, respectively. Then, the samples were subjected to isothermal annealing at 150, 220, 280 and 315 $^\circ C$, in steps of $\Delta t=60$ min. After each annealing step, IR absorption spectra were recorded by means of FTIR spectrometer (FTIR 470 plus) at LHT.

Fig.1 and Fig. 2 show segments of IR absorption spectra measurements and the evolution of the 1024 and 939 cm^{-1} absorption bands of the $C_iO_i(Si_i)$ defect, respectively. Upon annealing at 150 $^\circ C$, the above two bands decay and three new bands at 973, 952 and 724.5 cm^{-1} emerge. These three bands in turn, upon annealing at 220 $^\circ C$, are transformed into other three bands at 969, 951 and 977 cm^{-1} which are eliminated after 6 hours annealing at 280 $^\circ C$. Remarkably, the decay of this last group of bands is accompanied by the emergence of another two bands, at 1024 and 973 cm^{-1} . It is important to note that when the measurements are carried out at room temperature [4], the second group of band (at 973, 952 and 724.5 cm^{-1}) is not present in the spectra. Furthermore, from the three bands of the third group only two, that is 947 and 967 cm^{-1} , make their appearance [4].

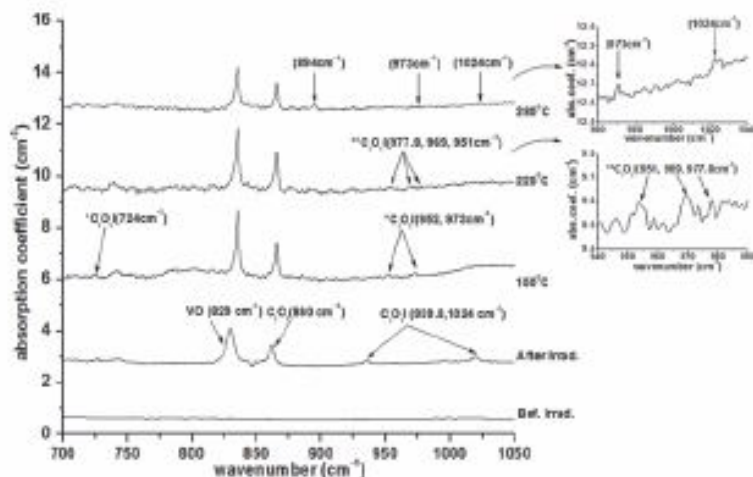


Figure 1: Segments of the IR absorption spectra in the range of 700-1050 cm^{-1} before and after irradiation as well as on thermal anneals at 150, 220 and 280 $^{\circ}\text{C}$ temperatures, for measurements at L.H.T.

Murin *et al.* [3] have proposed that the three groups of the bands correspond to different atomic configurations of $\text{C}_i\text{O}_i(\text{Si}_i)$ defects. In contrast to that, theoretical calculations predicted that the two later groups may originate from $\text{C}_i\text{O}_i(\text{Si}_i)_n$ complexes with $n > 1$ [5]. Apart from that, in neutron irradiated silicon the 947 and the 967 cm^{-1} bands have been attributed to $\text{C}_i\text{C}_i(\text{Si}_i)_2$ defects [6] because they appear in IR spectra simultaneously with the disappearance of the 987 993 cm^{-1} bands attributed to the $\text{C}_i\text{C}_i(\text{Si}_i)$ complex. Now, concerning the 1024 and 973 cm^{-1} bands, previous studies [4] have been proposed that the first band may correlate with the decay of 546 cm^{-1} band belonging to C_iC_i . In any case, the picture is not clear and any positive identification of the identity of these bands needs further investigation.

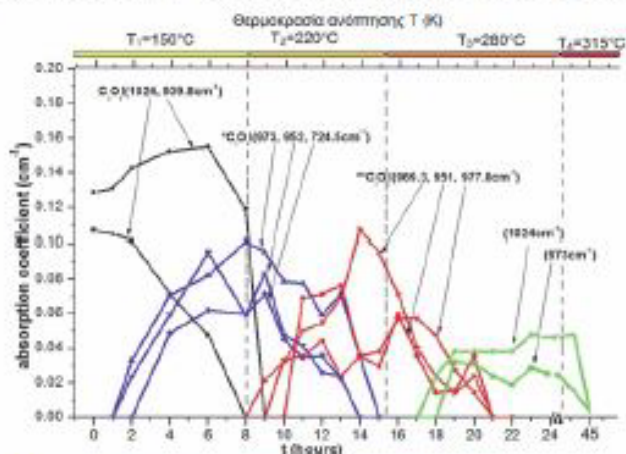


Figure 2: The evolution of $\text{C}_i\text{O}_i(\text{Si}_i)$ bands vs. annealing time, at 150, 220, 280 and 315 $^{\circ}\text{C}$ temperatures.

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