

## INTERSTITIAL BORON-INTERSTITIAL OXYGEN COMPLEX IN SILICON: LOCAL VIBRATIONAL MODE CHARACTERIZATION

L. I. Murin<sup>1</sup>, V. P. Markevich<sup>2</sup>, A. R. Peaker<sup>2</sup>

<sup>1</sup>*Scientific-Practical Materials Research Center of NAS of Belarus, Minsk 220072, Belarus*

<sup>2</sup>*The University of Manchester, Manchester M13 9PL, United Kingdom*

*E-mail: murin@ifftp.bas-net.by*

### INTRODUCTION

The interstitial boron–interstitial oxygen complex ( $B_iO_i$ ) is one of the dominant radiation-induced defects in oxygen-rich p-type Si crystals irradiated with MeV electrons at room temperature [1]. It is formed as a result of an interaction of mobile  $B_i$  atoms (generated via the Watkins replacement mechanism) with interstitial oxygen atoms. The  $B_iO_i$  defect appears to be a very efficient compensating center in irradiated p-Si and can affect the parameters of devices significantly since it removes a shallow acceptor ( $B_s$ ) and introduces a deep donor level at about  $E_C - 0.25$  eV. However, in spite of its technological importance the electronic properties of the  $B_iO_i$  center have not been understood properly, local vibrational modes (LVMS) of the defect have not been identified, and there is no consensus on its atomic structure. According to previous theoretical modeling studies [2] the  $B_iO_i$  complex can exist in several configurations with slightly different total energies. The electronic properties of the defect in these configurations are similar, but the LVMS appear to be different. An experimental observation of the  $B_iO_i$ -related LVMS may provide a solid basis for an unambiguous identification of the center.

### EXPERIMENTAL DETAILS

The samples used in the study were prepared from boron doped p-type Cz-Si crystals ( $\rho = 0.3\text{--}1 \Omega\cdot\text{cm}$ ). For a comparison a few samples from n-type Cz-Si crystals were studied as well. The concentration of interstitial oxygen was determined from measurements of absorption band at  $1107 \text{ cm}^{-1}$  using the calibration coefficient  $3.14 \times 10^{17} \text{ cm}^{-2}$  and was in the range  $(0.9\text{--}1.15) \times 10^{18} \text{ cm}^{-3}$  in both n- and p-Si.

Irradiations with 10 MeV and 6.0 MeV electrons were performed at room temperature with fluencies in the range  $1 \cdot 10^{16}\text{--}5 \cdot 10^{17} \text{ cm}^{-2}$ . Isochronal annealing was carried out in the temperature range 75–200 °C with 25 °C increments for 30 min at each temperature.

IR absorption analysis was carried out using a Bruker IFS 113v spectrometer. A spectral resolution of 0.5 or  $1.0 \text{ cm}^{-1}$  was used and the samples were measured at about 20 K (low temperature - LT), and at room temperature (RT).

## RESULTS AND DISCUSSION

Figure 1 shows fragments of absorption spectra in the range 525-1100  $\text{cm}^{-1}$  measured at 20 K for *p*- and *n*-type Cz-Si samples irradiated with 10 MeV electrons for a dose  $3 \times 10^{17} \text{ cm}^{-2}$  at RT. For the *n*-type Si all the observed radiation-induced LVM lines (spectrum 2) have been detected and identified previously. The main absorption band at 836  $\text{cm}^{-1}$  is related to the well known vacancy-oxygen defect (A-center). The minor bands located in the region of 865-1040  $\text{cm}^{-1}$  are associated with the interstitial type defects involving the Si self-interstitial (I), interstitial carbon ( $\text{C}_i$ ), and oxygen atoms [3, 4]. In particular, the well known band at 865  $\text{cm}^{-1}$  is related to  $\text{C}_i\text{O}_i$  complex, pairs of bands at 917, 1034  $\text{cm}^{-1}$  and 922, 1037  $\text{cm}^{-1}$  are associated with the  $\text{IO}_{2i}$  and  $\text{I}_2\text{O}_{2i}$  defects. The band at 936  $\text{cm}^{-1}$  has been assigned to an  $\text{I}_2\text{O}_i$  defect, while a pair of the bands at 939 and 1024  $\text{cm}^{-1}$  – to an  $\text{IC}_i\text{O}_i$  complex. The bands at 991 and 998  $\text{cm}^{-1}$  are related to  $\text{I}_3\text{C}_i\text{O}_i$  and  $\text{I}_2\text{C}_i\text{O}_i$  defects, respectively. The band at 648  $\text{cm}^{-1}$  is a combination mode arising from the single interstitial oxygen atoms.

Only very weak traces of the bands related to complexes involving the Si self-interstitial and/or  $\text{C}_i$  atoms can be detected in the spectrum of irradiated *p*-type Si. This observation indicates that there are some other traps, which are more efficient in capturing mobile radiation-induced I atoms than oxygen- and carbon-related centers, in this material and the appearance of some new complexes is expected. These complexes can give rise to vibrational absorption bands. Actually, as one can see in Fig. 1 (spectrum 1) in irradiated *p*-Si a new set of radiation-induced absorption lines is appearing. The most intense of them are positioned at about 538, 551, 688, 721, 756 and 991  $\text{cm}^{-1}$  (the later band cannot be related to the  $\text{I}_3\text{C}_i\text{O}_i$  defect since the other bands related to  $\text{I}_n\text{C}_i\text{O}_i$  are absent). All the bands are clearly observed also in the absorption spectrum measured at RT (Fig. 2). At room temperature the band positions are shifted to lower frequencies by about 3-5  $\text{cm}^{-1}$  and such shifts are typical for the LVMs due to radiation induced defects in silicon.

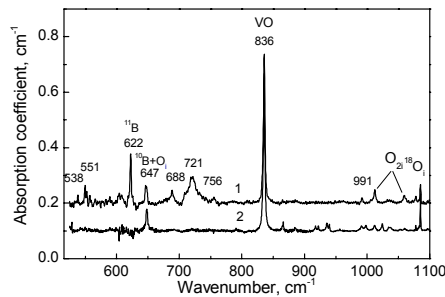


Fig. 1. Fragments of absorption spectra measured at 20 K for Cz-Si samples irradiated with 10 MeV electrons for a dose  $3 \times 10^{17} \text{ cm}^{-2}$ . 1 – *p*-Si ( $[\text{O}_i] = 1.0 \times 10^{18}$ ,  $[\text{C}_s] \leq 5 \times 10^{15}$ ,  $[\text{B}_s] = 8 \times 10^{16} \text{ cm}^{-3}$ ); 2 – *n*-Si ( $[\text{O}_i] = 1.15 \times 10^{18}$ ,  $[\text{C}_s] = 5 \times 10^{15}$ ,  $[\text{P}] = 6 \times 10^{14} \text{ cm}^{-3}$ )

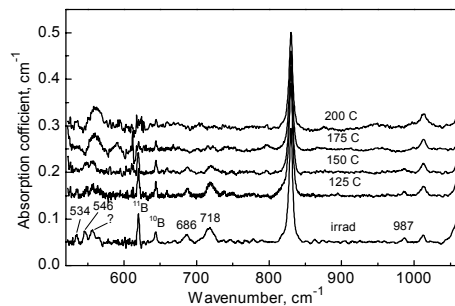


Fig. 2. Fragments of absorption spectrum measured at RT for *p*-Cz-Si sample irradiated with 10 MeV electrons for a dose  $3 \times 10^{17} \text{ cm}^{-2}$  and then subjected to isochronal anneals with the last steps at the temperatures indicated above the curves

It should be mentioned that the same set of the LVM bands was detected also in the irradiated samples with a lower boron content ( $\rho = 0.5\text{-}1 \Omega\cdot\text{cm}$ ), but the intensities of the bands in these samples were lower than those in the samples with  $\rho = 0.3 \Omega\cdot\text{cm}$ . This finding suggests an involvement of boron atoms in the composition of the center responsible for the bands. According to earlier studies, irradiation of Si samples with low oxygen and high boron content did not result in an appearance of the boron-related bands mentioned above and observed by us in the oxygen rich samples. The later fact indicates the presence of oxygen atoms in the center giving rise to a new set of the LVM bands. It seems reasonable to suggest that this center is a  $\text{B}_i\text{O}_i$  defect. Such an assignment is supported by the results of the thermal stability study of the bands observed.

Figure 3 shows the development of the IR absorption spectra measured at low temperature for an irradiated *p*-Cz-Si sample after 30-minutes isochronal annealing steps in the temperature range 100-200 °C. Upon annealing up to 150 °C there are no essential changes in the spectra. However, after annealing at 175 °C the situation changes drastically. All the new lines are not observed any more, a strong increase in the absorption by free holes does occur and a number of new rather strong peaks and dips are appearing. The peaks positioned at about 668, 693 and 702  $\text{cm}^{-1}$  are related to transitions of holes from the boron ground  $1s$  state in the forbidden gap to the excited  $2p'$ ,  $3p'$  and  $4p'$  states associated with the split-off  $p_{1/2}$  valence band. A set of profound dips positioned at 521, 703, 765, 782 and 798  $\text{cm}^{-1}$  are due to resonant interaction of optical phonons with acceptor continuum states [5].

It should be mentioned that a strong absorption by free holes and the presence of intense peaks and dips related to electronic transitions do not allow to make a definite conclusion that all the new relatively weak LVM lines disappear simultaneously upon annealing at 175 °C. However, an analysis of the spectra measured at RT (see Fig. 2) shows that such disappearance actually does occur. Thus, the thermal stability of the defect giving rise to a set of new LVM lines and a partial recovery of the free hole concentration observed upon its annihilation are consistent with the similar features known for the  $\text{B}_i\text{O}_i$  defect [1, 2].

### CONCLUSION

FTIR spectroscopy was used to study the boron- and oxygen-related defects in Cz-grown *p*-type Si samples irradiated with fast electrons at RT. A set of new LVM lines with the same formation and elimination behaviors has been observed. The most intense lines of the set are found to be at 991, 721 and 550  $\text{cm}^{-1}$ . On the basis of an analysis of changes in intensity of the lines with content of impurities and annealing temperature the lines have been assigned to the LVMs of the  $\text{B}_i\text{O}_i$  defect.

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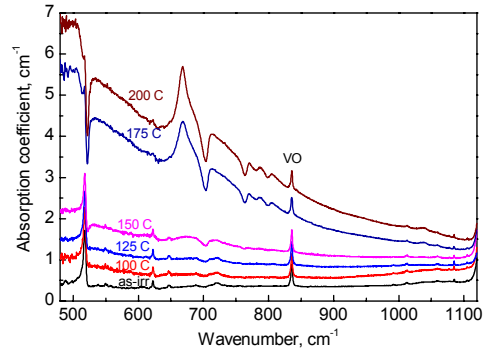


Fig. 3. Development of the IR absorption spectra measured at 20 K for the *p*-Cz-Si sample used in Fig. 1 after isochronal annealing steps in the temperature range 100-200 °C

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