Boron - Oxygen Interaction in Boron-Doped Czochralski Grown Silicon

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A new electrically active defect is revealed in Si:B samples. An additional linear absorption in the region of the intracenter absorption for boron is associated with the defect. The energy distance between the spectral lines is in good agreement with the predicted by the effective mass theory for acceptors of group III in Si. The defect associated with the line is identified as B_sO_{2i}* owing to the linear dependence of its formation efficiency on the boron content and the quadratic dependence on the oxygen concentration. The revealed absorption lines correspond to the intracenter transitions from the ground to the excited states of boron, which are shifted relative to the main transitions due to a deformation perturbation from two neighbouring oxygen atoms. The defect is formed both during the growth of silicon and under the action of elevated temperatures. It is supposed, boron atom in the structure of revealed B_sO_{2i}* defect forms direct bonds with two neighbouring oxygen atoms.

It is found that at elevated temperatures the detected B_sO_{2i}* defect transforms into a new state, which is associated with the emergence of the additional absorption line in the range of intracenter transitions for boron. A strong correlation was registered between the increase in the intensity of new absorption component with the temperature and the decrease in the intensity of the line associated with the B_sO_{2i}*. It is suggested that there is the temperature-induced transformation of the local atomic configuration of the B_sO_{2i}* complex. The activation energy of the B_sO_{2i}* transformation into a new configuration is 2.59 eV.

The data obtained testify that the BO_2 defects with different structure and properties can be formed in boron-doped Si and must be taken into account when developing Si:B-based devices.

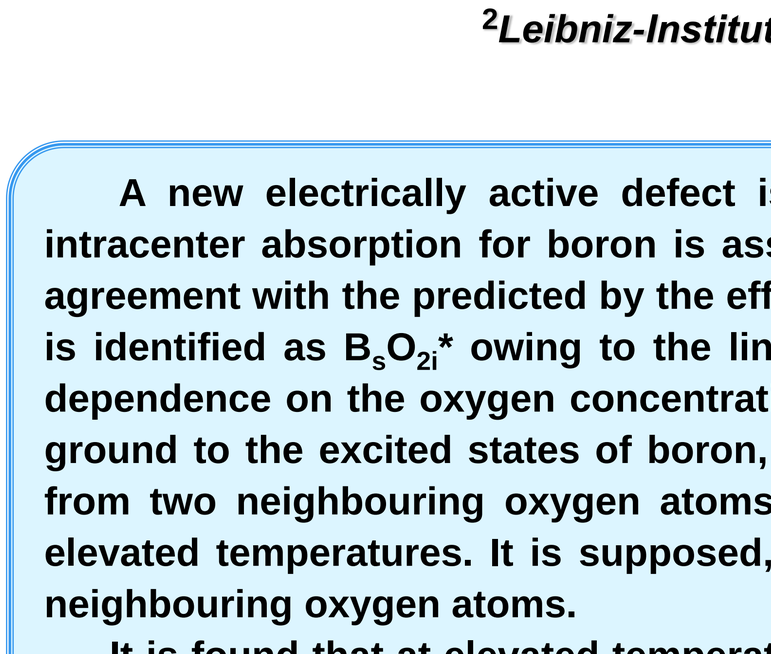

Fig. 1. **Absorption spectra measured at 10 K for the as-grown boron-doped Cz-Si sample (a) and subjected to heat treatment at 400 ºC for 10 h (b). N_B = 2,2×10¹⁶ cm⁻³. N_O = 1,09×10¹⁸ cm⁻³. The identification of boron transitions is shown at the top. Spectrum (b) is multiplied by 2. The spectra are baseline corrected and shifted along the vertical axis for clarity.**

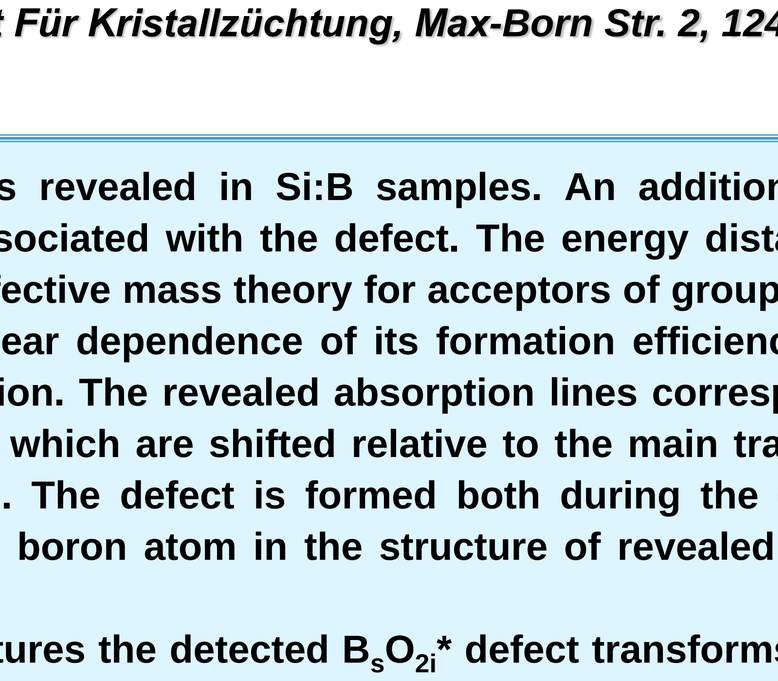

Fig. 2. **Intensity of the 261,3 cm⁻¹ absorption line as a function of oxygen (a) and boron (b) content in the samples Cz-Si:B. $T_{ann.}$=400 ºC for 10 h. The points correspond to the experimental data. The solid line is fitted to the measured data.**

***Table 1.* Comparison of the energy spacing (meV) between the transitions $1\Gamma_8^+ \rightarrow 1\Gamma_8^-$ and $1\Gamma_8^+ \rightarrow 2\Gamma_8^-$ for boron as calculated by the effective mass theory (EMT) with the measured spacing between these transitions for boron and the lines revealed in heat-treated Cz-Si:B.**

Boron, experimental	B_sO_{2i} defect	EMT[a]	EMT[b]
4,12	4,13	4,09	4,1

[a] R. Buczko and F. Bassani, Phys. Rev. B 45, 5838 (1992).
[b] N. O. Lipari, A. Baldereschi, and M. L. W. Thewalt, Solid State Commun. 33, 277 (1980).

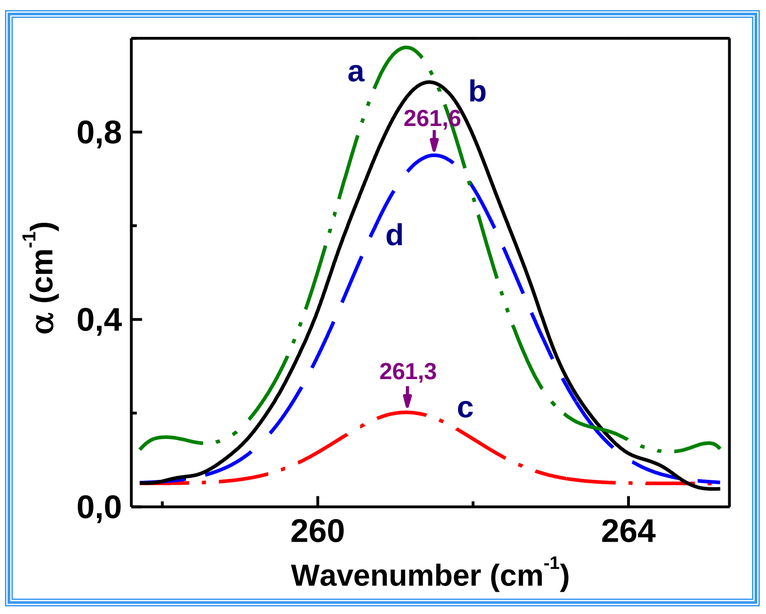

Fig. 3. **Fragments of the absorption spectra measured at 10 K with the resolution 0,2 cm⁻¹ for Cz-Si:B sample annealed at 400 ºC for 10 h (spectrum a) and subjected to the subsequent heat treatment at 540 ºC for 30 min (spectrum b). Decomposition of the spectrum (b) into components (c, d) is shown. N_B=2.2×10¹⁶ cm⁻³, N_O=1×10¹⁸ cm⁻³. The spectrum (a) is multiplied by 0,5 for clarity.**

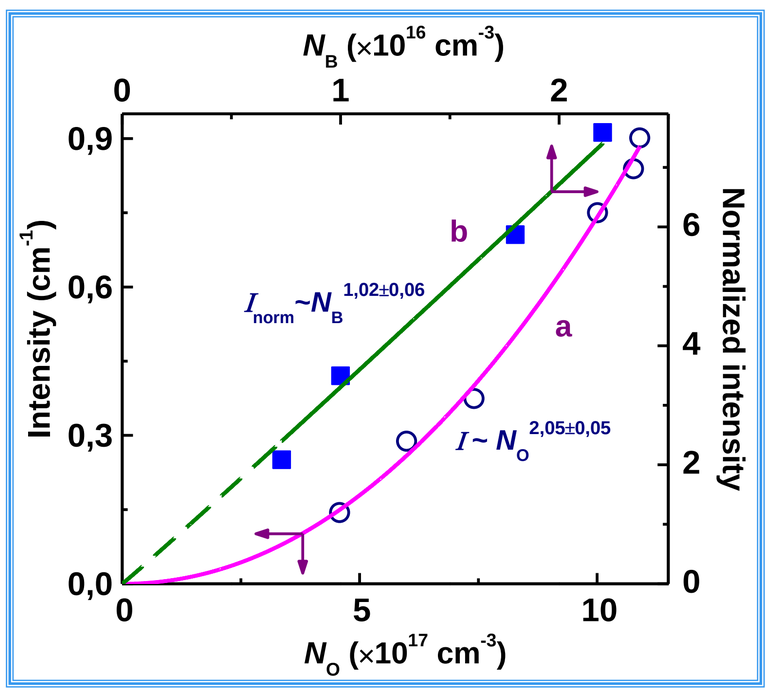

Fig. 4. **Intensity of the 261,6 cm⁻¹ absorption line as a function of oxygen (a) and boron (b) content in the samples Cz-Si:B. $T_{ann.}$=540 ºC for 30 min. The points correspond to the experimental data. The solid line is fitted to the measured data.**

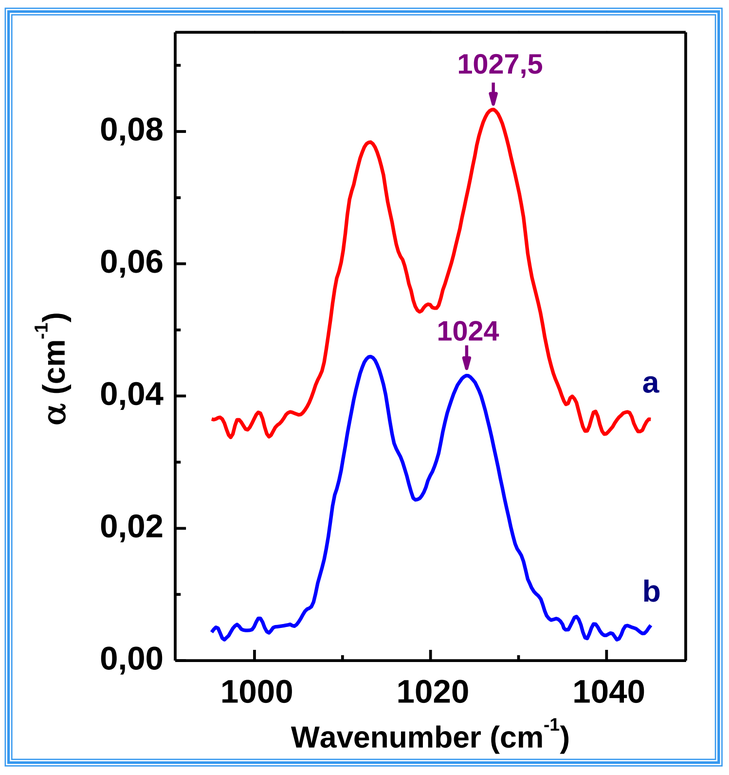

Fig. 5. **Fragments of the absorption spectra measured at room temperature for boron-doped Cz−Si sample annealed at 500 ºC (a) and 530 ºC (b). Time of heat treatments t_{ht}=60 min. N_B=2,2×10¹⁶ cm⁻³. N_O=1,12×10¹⁸ cm⁻³.**

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