Boron - Oxygen Interaction in Heat Treated Silicon

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Summary

The influence of heat treatment at 400 ºC on the spectrum of boron intracenter transitions in silicon using IR absorption spectroscopy is investigated. In the transitions region from the ground $1\Gamma_8^+$ state associated with the $p_{3/2}$ valence band of Si to the odd-parity excited states of boron, a new absorption line with its maximum at 261.3 cm^{-1} is observed in the thermally treated boron-doped Cz-Si. Oxygen is a component of defect that is responsible for the detected absorption line. Perturbation of boron atoms due to the inhomogeneous stress effect from neighboring oxygen atoms results in a frequency shift in the main boron transition. The defect associated with 261.3 cm^{-1} line is also observed in as-grown silicon. The defect disappears during annealing at 550 ºC. The estimated concentration of the detected defect for the as-grown and heat treated at 400 ºC during 10 h Cz-Si:B sample (N_B=2.2×10^{16} cm^{-3}; N_O=1.1×10^{18} cm^{-3}) are 7.8×10^{12} cm^{-3} and 1.7×10^{14} cm^{-3}, respectively. The binding energy of the $1\Gamma_8^+$ ground state for revealed defect is 43.93 meV.

The acquired data are essential for understanding the influence of boron-oxygen-related defects on the electrical and optical properties of silicon and photovoltaic cells made on its base.

Experimental

The samples of boron-doped Si used in the study were grown by the Czochralski (Cz-Si:B) and float-zone (Fz-Si:B) methods. The concentration of boron (N_B) was 1×10^{16} and 2.2×10^{16} cm^{-3} for Cz-Si:B samples and 2.6×10^{16} cm^{-3} for Fz-Si:B. The content of oxygen (N_O) was changed in samples in the range (0.43÷1.1)×10^{18} cm^{-3}. The carbon concentration was varied in the interval (0.8÷1.2)×10^{17} cm^{-3}. To study the interaction between boron and oxygen atoms the heat treatments of samples were carried out at 400 ºC during 10 h. The absorption spectra of the samples were studied with the use of a Bruker IFS-113v Fourier transform infrared spectrometer. The measurements were carried out at 10 K with a resolution of 0.2−1 cm^{-1}.

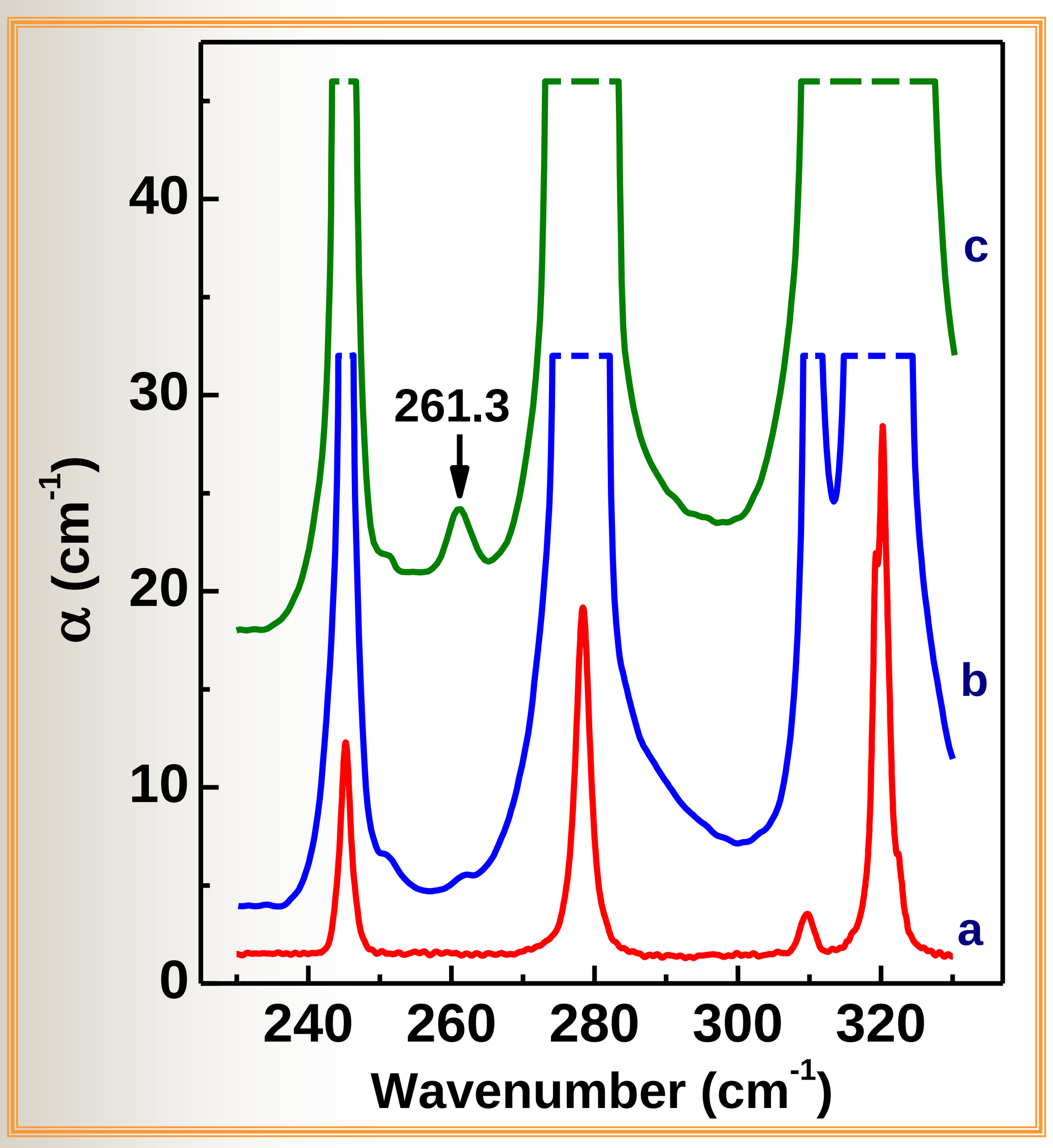

Fig. 1. **Infrared absorption spectra measured at 10 K for the Cz-Si:B. N_B, ×10^{16} cm^{-3}: a − 0.04; b, c − 2.2. N_O, ×10^{18} cm^{-3}: a − 1; b, c − 1.1. Spectrum (c) corresponds to the sample heat treated at 400 ºC for 10 h. The spectra are shifted along the vertical axis for clarity.**

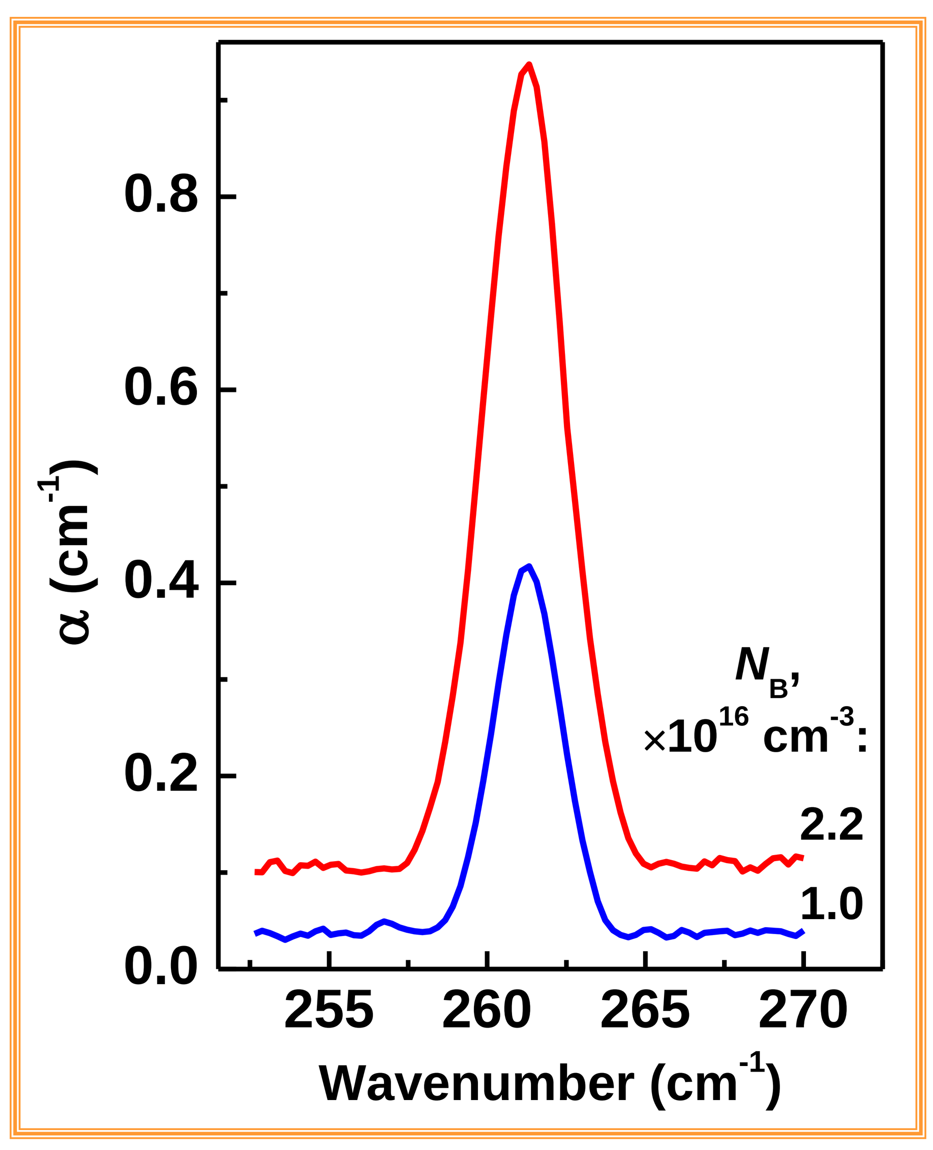

Fig. 2. **Fragments of the absorption spectra for the Cz-Si:B samples with comparable oxygen concentrations (N_O~4.5×10^{17} cm^{-3}) and different boron contents. Samples heat treated at 400 ºC for 10 h. The spectra are baseline corrected.**

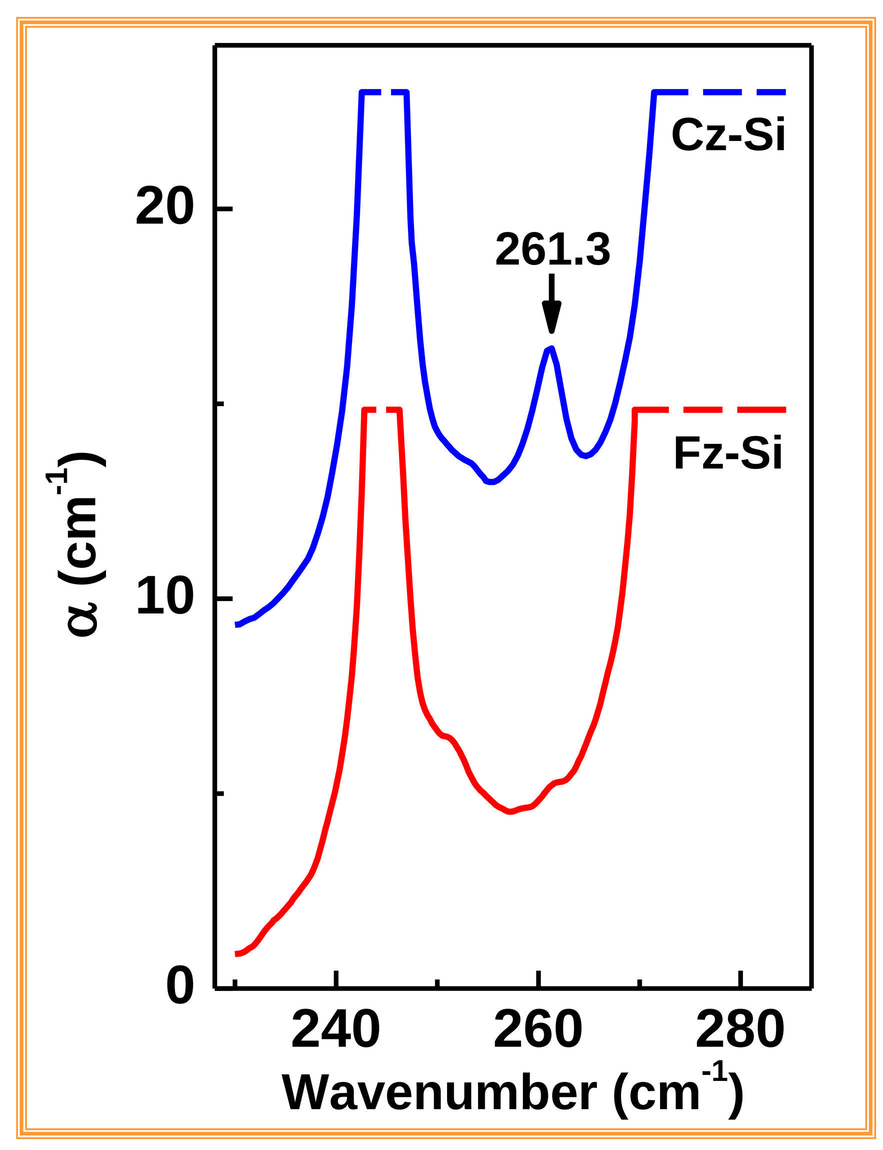

Fig. 3. **Fragments of the absorption spectra for Fz-Si:B (N_B=2.6×10^{16} cm^{-3}; N_O= ≤3×10^{15} cm^{-3}) and Cz-Si:B (N_B=2.2×10^{16} cm^{-3}; N_O=1.08×10^{18} cm^{-3}) samples heat treated at 400 ºC for 10 h.**

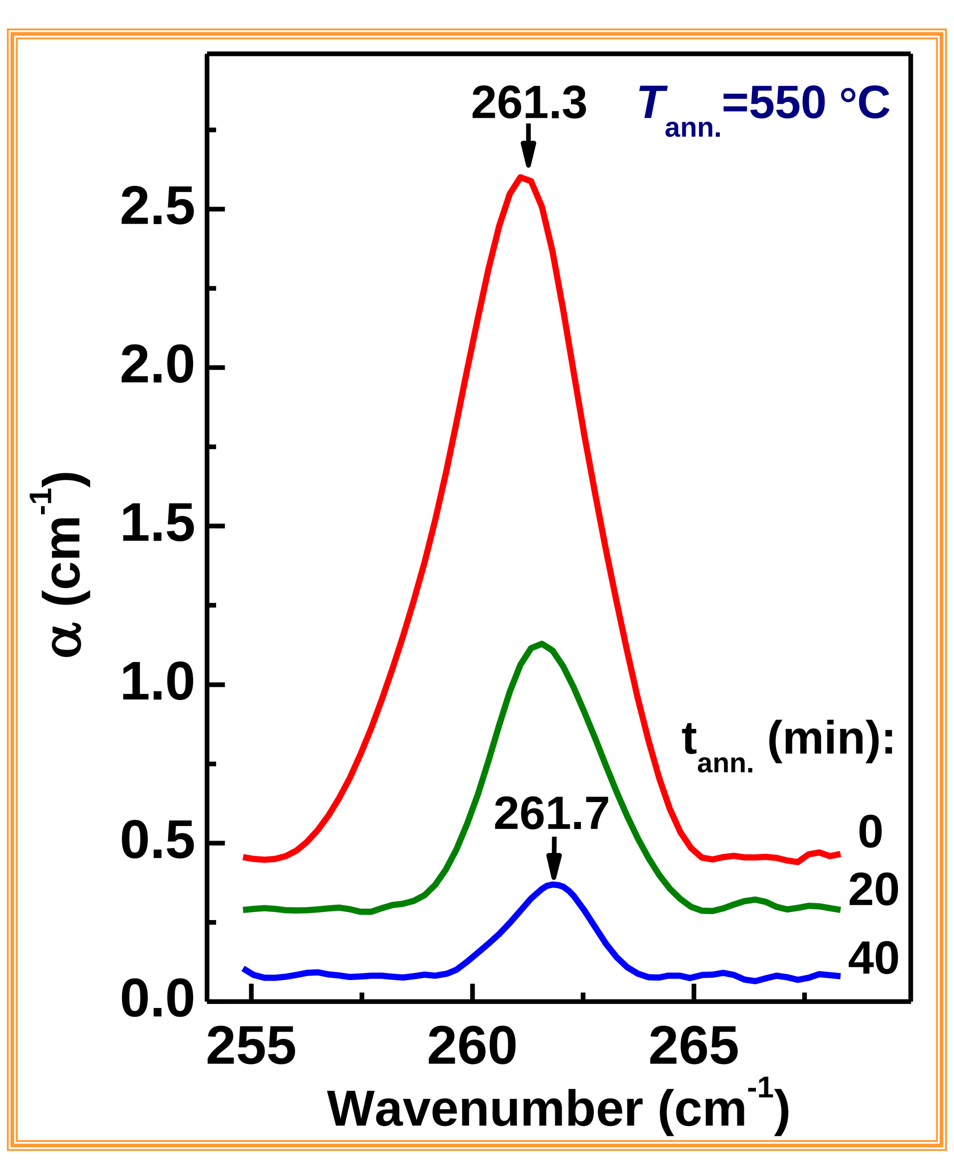

Fig. 4. **Fragments of the absorption spectra for boron-doped Cz-Si sample heat treated at 400 ºC for 10 h and subjected to the subsequent annealing at 550 ºC. N_B=2.2×10^{16} cm^{-3}. N_O=9.3×10^{17} cm^{-3}.**

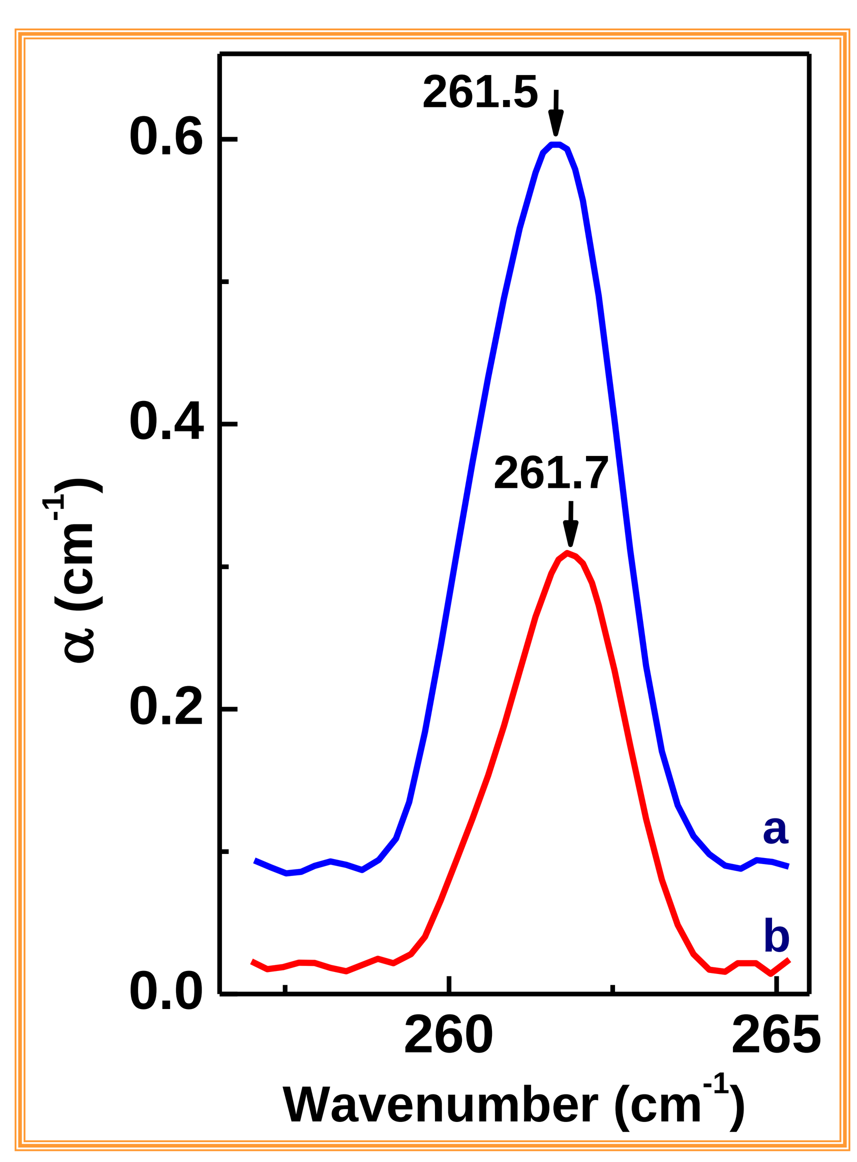

Fig. 5. **Fragments of the absorption spectrum for as-grown Cz-Si:B sample (a) and after its successive heat treatments at 400 and 550 ºC (b). N_B=2.2×10^{16} cm^{-3}. N_O=1.02×10^{18} cm^{-3}.**