TEMPERATURE-DEPENDENT CHANGE OF SITE OCCUPANCIES IN BORON CARBIDE

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Behind diamond, cubic boron nitride and boron suboxide, boron carbide is the forth-hardest material known. It's Mohs Hardness is 9.3 and the Vickers Hardness >30 GPa. This confirms high bond strength within the structure. Nevertheless, several studies indicate that regular atoms in the structure are able to change their sites already at moderate temperatures.

Aside from self-healing processes in boron carbide [1], Lezhava et al. [2] reported on six internal friction maxima between 115 and 750 K. Yao et al. [3] predicted theoretically an exothermic phase transition between 717 and 790 K, attributed to the site exchange of carbon atoms within the icosahedra. Using specific heat measurement, Werheit et al. [4] found an endothermic phase transition at 712 K. Negative Grüneisen parameters of specific phonons [5] support the assumption that the central B atom in the three-atomic chain buckles out under pressure [6,7]

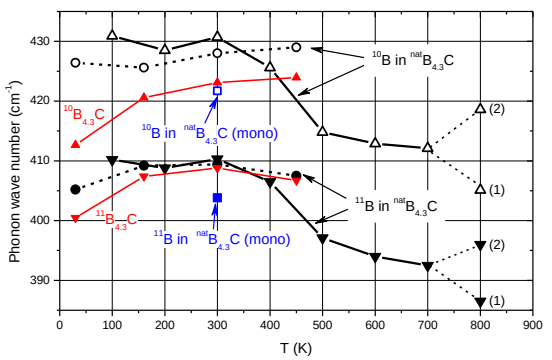

Fig. 1. Temperature dependence of the isotope-related components of the IR-active phonon near 400 cm^{-1}

Phonon spectra have proven to yield valuable information on the boron carbide structure. The IR-active phonon near 400 cm^{-1} is related to the central B(3) atom vibrating perpendicular to the axis of the three-atomic chain .

In the spectrum, ^{10}B and ^{11}B components are clearly distinguishable. The temperature dependence (Fig. 1), exhibits two significant features: phonon softening below 300 K and splitting between 700 and 800 K. The latter is obviously related to the phase transition [4].

Below ~400 K, the ^{10}B/^{11}B relation 19/81 in ^{nat}B determines the B(3) occupancy Towards higher temperatures, this relation changes significantly and reaches nearly equal values near 800 K, thus indicating that the isotopes change atomic sites.

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