ISOTOPE EFFECT IN THE RAMAN SPECTRA OF $Li_2B_4O_7$ SINGLE CRYSTALS

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S u m m a r y

The Raman spectra investigations are performed at room temperature in the range 100–1200 cm^{-1} for $Li_2B_4O_7$ single crystals grown by the Crochralsky technique with natural isotope distribution of Li and B, as well as 4 variants of single crystals maximally enriched by ^7Li, ^6Li, ^{10}B, and ^{11}B isotopes. The specific modes are divided conditionally into 5 groups by the frequency changes: 1) 'regular“ modes, for which the frequency of a vibrational mode decreases when the substitution by an isotope with larger mass takes place; 2) modes practically insensitive (within the limits of the frequency measurement accuracy) to the substitution of any isotope; 3) modes with anomalous frequency behavior, when the frequency of a vibrational mode decreases at the substitution by an isotope with smaller mass; 4) modes with unforeseen chaotic changes of frequency at the isotope substitution; 5) 'accidental“ modes, which are observed only in some samples. Consequently, the modes of the first group are related to the fundamental modes of the crystal. The modes of the second group (high-frequency modes) are connected with vibrations of the oxygen atoms that are located in 4 nonequivalent positions of the $Li_2B_4O_7$ lattice, while the low-frequency ones – with probable plasma vibrations. The third and fourth groups of the modes are caused, without doubt, by the frequency mixing of different modes (valent, deformational, and librational) of different boron-oxygen groups with one another, and by lithium clusters. Local vibrations within the limits of the isolated defects of the lattice, especially, impurities, can be a reason for the appearance of peeaks from the fifth group. In result, from the analysis the frequency shifts for separate vibrational modes at the substitution of isotopes ^7Li to ^6Li and ^{11}B to ^{10}B, the identification of some fundamental vibrational modes is corrected. It is found that isotope splitting does not take place in the Raman spectra of single crystals with the natural isotope distribution, this fact indicates the exclusively one-mode behavior for isotopically mixed $Li_2B_4O_7$ crystals. It is ascertained that almost a half of modes that are observed in the Raman spectra of $Li_2B_4O_7$ single crystals, belongs to the mixed vibrations of various types, which is connected with the frame structure of the crystalline lattice consisting of complex boron-oxygen groups.

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