

Unexpected concentration dependence of Ba²⁺ dominant substitution in addition to La³⁺ in cubic Nd³⁺-doped BaLaLiWO₆ perovskites

Autorzy

Kacper Albin Prokop

E. Tomaszewicz

Miłosz Siczek

Y. Guyot

G. Boulon

Małgorzata Guzik

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There is a great need in material science to find and investigate new RE³⁺ ion-doped inorganic materials suitable for producing sintered ceramics of high transparency. Prospective candidates for transparent ceramics should crystalize in highly symmetric crystal systems, so BaLaLiWO₆ characterized by a cubic structure (s.g.) seems to be a good candidate for accomplishing this highly challenging task. A series of micro-crystalline samples activated by Nd³⁺ ion (0–20 mol%) was produced *via* the solid-state reaction. Nd³⁺ ion was chosen as a laser dopant and structural probe. For the first time, the BaLaLiWO₆ crystal structure was solved from the single crystal. The originality of this research results from the unexpected substitution of divalent Ba²⁺ ions by trivalent Nd³⁺ ones till up to 7 mol% and above this value the replacement of probably both Ba²⁺ and La³⁺ ions. Exchange of Ba²⁺ by Nd³⁺ ions leads to the formation of cationic vacancies due to the charge compensation effect: 3Ba²⁺ → 2Nd³⁺ + □ (vacancy in La³⁺ cationic sublattice), well-manifested in unit cell expansion with consequences in the spectroscopic characteristics. XRD and SEM methods in combination with emission and absorption spectroscopic ones used at cryogenic temperature helped to determine the substantial properties of this perovskite which could find application in optics. Slightly different cationic positions substituted by the Nd³⁺ ion and its non-homogeneous arrangement in the Ba²⁺/La³⁺ site, detected by spectroscopy with selective excitation under laser at 77 K, is pointed out. The crystal disorder of the cation environment is revealed in broad absorption and emission bands even at low temperature.

Słowa kluczowe

Perovskite-type tungstates, Cubic BaLaLiWO₆, Nd³⁺ structural probe, Cationic vacancy, Optical materials

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