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Crystal Electric Field Effects and Thermal Expansion of Rare-Earth

Hexaborides

V.V. Novikov¹*, E.S. Pilipenko¹, S.L.Bud'ko²

¹Training-Research Center "Bryansk Physical Laboratory", Petrovsky Bryansk State University 14, Bezhitskaya St, 241036 Bryansk, Russia

²Ames Laboratory U.S. DOE, and Department of Physics and Astronomy, Iowa State University, Ames, IA, 50011, USA

*Corresponding author. E-mail: vvnovikov@mail.ru

Abstract

Anomalies in the magnetic contribution to the thermal expansion coefficients $\Delta\beta(T)$ of the CeB₆, PrB₆, and NdB₆ hexaborides in the range of 5-300 K were found by comparison with diamagnetic LaB₆. The characteristic of the anomalies was the same in all the studied borides: a distinct peak at low temperatures, followed by a broad maximum at higher temperatures (50–100 K), then a decrease and transition to the region of negative values as the temperature increases further. The features of $\Delta\beta(T)$ are explained by the effects of the magnetic order (sharp low temperature peaks) and the crystal electric field (CEF). The $\beta_{CFF}(T)$ dependencies were calculated using Raman and neutron scattering data on the splitting of the rare-earth (RE) ions R^{3+} f-level by the CEF. A satisfactory consistency between the values of $\beta_{CEF}(T)$ and $\Delta\beta(T)$ was obtained for the studied hexaborides. Additionally, we determined the values of the Grüneisen parameter γ_i that correspond to the transition between the ground and excited multiplets of R³⁺ ions f-level splitting.

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