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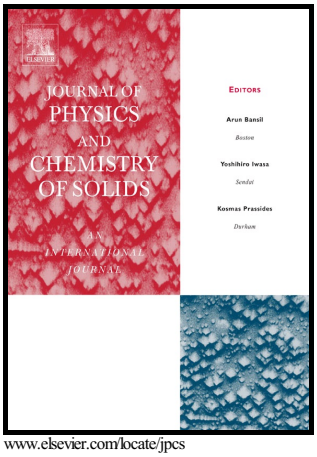

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Two-Level Systems and Negative Thermal Expansion of Lutetium Borides

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Abstract.

The heat capacity $C_v(T)$ and unit cell volume V(T) temperature dependencies of lutetium borides LuB_2 and LuB_4 in the region of 2–300 K were analysed in the Debye-Einstein approximation. The characteristic temperatures of the Debye and Einstein components of boride heat capacity and thermal expansion were found. The anomalous contribution to the borides' thermal characteristics was revealed. This contribution was attributed to the influence of two-level systems (TLS), formed in the subsystem of lutetium ions due to asymmetry in the way they are surrounded by the boron atoms in the boride crystal structure. The TLS influence is revealed on heat capacity temperature dependencies by the Schottky-type maxima at $T_{max\ LuB2}$ =13.8 K, $T_{max\ LuB4}$ =22.7 K, as well as by the negative contribution to the borides' thermal expansion. The borides' Grüneisen parameters corresponding to the heat capacity and thermal expansion TLS anomalies are negative, and amount to several 10s of units.

Keywords: borides, heat capacity, thermal expansion, two-level systems.

1. Introduction

Rare-earth borides attract workers due to their wide scope of rather interesting physical and physicochemical properties, including superconductivity, magnetic, structural and phase transitions, and peculiar dependencies of physical property temperature changes over a wide range of low and high temperatures [1–10].

One of the features of some rare-earth borides is the negative thermal expansion at low temperatures. This phenomenon is accompanied by the anomalous behaviour of the borides' heat