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Theoretical investigation of structural, electronic and mechanical properties of the hard LaB_4 material

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ABSTRACT

This study investigates the structural, electronic, elastic and dynamic properties of the lanthanum tetraboride through Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT), using the Generalized Gradient Approximation (GGA), Local Density Approximation (LDA) and Local Density Approximation plus Hubbard (LDA + U) exchange-correlation potentials. The obtained lattice constants and atomic positions are in good agreement with the available data presented in literature. The band structure illustrated that LaB_4 is a conductor and the partial density of states and electronic localization function (ELF) analysis indicated the existence of covalent character in B–B and B–La bonds, which indicate that this material is an intermetallic in nature. We discussed the physical significance of the obtained elastic constants, stress-strain relations and the other relevant quantities, such as shear, bulk and Young's moduli, Poisson's ratio, hardness, and Debye temperature. The results revealed that the lanthanum tetraboride is mechanically stable, brittle, hard and anisotropic. Finally, we estimated the thermodynamic properties such as the Helmholtz free energy, internal energy, entropy and specific heat capacity in the 0–2000 K temperature range, within the phonon-dispersion and the phonon density of states curves.

1. Introduction

The technological uses of superhard materials have considerably attracted the scientific community and industrials due their various interesting electronic and mechanical properties. A few of these materials are eligible to be refractory materials, thermionic emitters, and steel alloying agents [1–4]. Many researchers have discovered the superconductivity in some of these compounds, such as MgB_2 and Li–P–B ternary boride [5,6].

The most of superhard materials are composed of light elements (B, C, N and O), like c-BN, BC_2N and diamond. Therefore, the hardness of these compounds is mainly due to the short and strong covalent bonds between these elements, which make it resist plastics deformations. Unluckily, these types of materials are expensive, very rare in nature and need to be synthesized under high-level pressure and extreme high-temperature conditions [7]. Consequently, huge research efforts are consecrated in designing new superhard materials; among the methods used, we can distinguish carbides, nitrides and also the borides of transition metals, rare earth or actinides which are promising approaches in the conception of those superhard materials [2,8–10].

The carburizing of these materials has been widely studied such as nanotubes, graphite linked materials, etc. On the other hand, metal borides are still an important field to be exploited. These compounds form an interesting class with a large range of technological applications [11]. This explains the efforts made during these last five decades in the field of borides of transition metals and lanthanides. The rare earths tend to form boron-rich materials, contrary to transition metals which form metal-rich phases, as diborides (REB_2), tetraborides (REB_4), hexaborides (REB_6), and dodecaborides (REB_{12}) [12–14]. These compounds have good physical properties such as high melting points, high hardness

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