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FIRST-PRINCIPLES STUDY ON MECHANICAL PROPERTIES OF THE PEROVSKITE RBRh_3 ($\text{R} = \text{Sc}, \text{Y}$ AND La) ALLOYS

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Abstract : The structural, elastic and thermodynamic properties of the cubic perovskite RBRh_3 ($\text{R}=\text{Sc}, \text{Y}$ and La) compounds have been calculated using the full-potential linearized-augmented plane wave with the mixed basis FP/APW+lo method. The exchange-correlation potential is treated with the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE). The calculated structural properties are in excellent agreement with the available experimental and theoretical data. Single-crystal elastic constants are calculated using the total energy variation with strain technique, then the shear modulus, Young's modulus, Poisson's ratio and anisotropic factor are derived for polycrystalline RBRh_3 . Ductility behaviour of these compounds is discussed via the elastic constants C_{ij}

Keywords : Perovskite borides; ab initio calculations; Elastic constants.