The 3rd International Conference on welding, nondestructive testing and the industry of materials and alloys (ICWNDT-MI'12)

2012

FIRST-PRINCIPLES STUDY ON MECHANICAL PROPERTIES OF THE PEROVSKITE RBRh3(R = Sc, Y AND La) ALLOYS

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Abstract : The structural, elastic and thermodynamic properties of the cubic perovskite RBRh3 (R=Sc, 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 odulus, Young's modulus, Poisson's ratio and anisotropic factor are derived for polycrystalline RBRh3. Ductility behaviour of these compounds is discussed via the elastic constantsij C

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