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Structural and Physical Properties of DyCu, NdAg, LaCd, YIn, ErCu, ErAg, and ErAu Rare-Earth Intermetallic Compounds: *Ab-Initio* Investigations Analyzed by Data Mining Technique

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In this work, the structural, elastic, mechanical, thermodynamic, and electronic properties of ErCu, ErAg, ErAu, DyCu, NdAg, LaCd, and YIn compounds have been investigated systematically using full-potential linearized augmented plane wave (FP-LAPW) within the density functional theory (DFT). In this approach, the exchange–correlation energy was calculated with generalized gradient approximation (GGA), by Perdew–Burke–Ernzerhof (PBE). We have firstly calculated lattice constants, bulk modulus, elastic constants, and mechanical properties such as Young's and shear moduli, Pugh factor (B/G), anisotropy constant, and Cauchy pressure, as well as Poisson coefficient. The elastic constants and their related properties verify the criteria of mechanical stability, signifying that these compounds are stable in B2 structure. The ductility of the intermetallics investigated here is evaluated. The obtained values show that ErCu is the most rigid while NdAg the most ductile. The total and partial electron density of states (DoS) were evaluated to offer a detailed explanation of the contribution of atomic orbitals in the energy bands. The thermodynamic properties of ErCu, ErAg, ErAu, NdAg, LaCd, YIn, and DyCu are calculated via the quasi-harmonic Debye model, in which the lattice vibrations are considered. So temperature-dependent parameters such as lattice constant, thermal expansion, and specific heat at constant volume are analyzed. Furthermore, the relationship between several thermo-physical and mechanical properties was discussed and analyzed with data mining techniques. The obtained results confirm that this B2-type of rare-earth intermetallics has very interesting mechanical and thermal properties for structural applications.

Keywords: rare-earth intermetallic phases, *ab-initio* calculations, elastic and mechanical properties, thermodynamic properties, density of states (DoS), data mining method.