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Electronic and high pressure elastic properties of RECd and REHg (RE=Sc, La and Yb) intermetallic compounds

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ABSTRACT

Structural, electronic, elastic and mechanical properties of Cd and Hg based rare earth intermetallics (RECd and REHg; RE=Sc, La and Yb) have been investigated using the full-potential linearized augmented plane-wave (FP-LAPW) method within the density-functional theory (DFT). The ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') have been obtained using optimization method and are found in good agreement with the available experimental results. The calculated enthalpy of formation shows that LaHg has the strongest alloying ability and structural stability. The electronic band structures and density of states reveal the metallic character of these compounds. The structural stability mechanism is also explained through the electronic structures of these compounds. The chemical bonding between rare earth atoms and Cd, Hg is interpreted by the charge density plots along (1 1 0) direction. The elastic constants are predicted from which all the related mechanical properties like Poisson's ratio (σ), Young's modulus (E), shear modulus (G_H) and anisotropy factor (A) are calculated. The ductility/brittleness of these intermetallics is predicted. Chen's method has been used to predict the Vicker's hardness of RECd and REHg compounds. The pressure variation of the elastic constants is also reported in their B_2 phase.

1. Introduction

During last few decades, the properties of lanthanide intermetallic compounds have been extensively investigated from the point of view of applications as well as fundamental research. Due to the presence of partially filled f electron orbital, these compounds show many peculiar physical properties. To the date rare earth intermetallic compounds have found their niche in a range of applications from superconductors, permanent magnets, catalysts and electrocatalysts and hydrogen storage systems as well as, in some cases, promising structural materials [1]. Intermetallic compounds are among the most important solid state materials because of their diverse physical properties and widespread use in numerous applications. Intermetallics received great attention due to their unique mechanical properties, such as high tensile strength, good ductile/brittle behaviour, high corrosion resistance and thermal stability [2–8]. In intermetallic compounds the absence of 'd' like electrons in the vicinity of the Fermi level (E_F) accounts for the observed ductility in 90% of the compounds [9]. A well-known property of the rare earth elements is their incomplete 4f shell, which becomes progressively filled in going from La to Lu. The shielding of the 4f shell leads to interesting physical properties which differ from one lanthanide ion to the next by the number of electrons compacted in the 4f shell.

Rare earth based intermetallics RECd and REHg (RE=Sc, La and Yb) are binary intermetallic compounds with CsCl structure, which belong to *Pm3m* space group (no 221). Indelli et al. [10] have predicted that these compounds are stable in B_2 phase and calculated the lattice parameters at ambient conditions by using X-ray diffraction technique. Apart from the experimental lattice parameter on these intermetallics no systematic experimental or theoretical results on the elastic, mechanical and electronic properties are available in literature. RECd and REHg intermetallic compounds have gained attention as reference materials; Sc has only single 3d electron in its outermost orbital, La atom has unoccupied 4f orbitals while Yb has fully filled 4f orbitals in its outermost shell. In the present paper a comprehensive and systematic study related to the ground state, electronic, elastic and thermal properties for these compounds has been carried out in. An ab-initio investigation of structural, elastic, electronic, lattice dynamical and thermodynamic properties of ScZn and

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YZn in the B_2 structure has been reported by Soyalp et al. [11]. Thermal stabilities, elastic properties and electronic structures of MgSc, MgY and MgLa have been determined by Chen et al. [12] from first-principles calculations. Full-potential linearized augmented plane wave (FLAPW) method has been employed within the generalized gradient approximation (GGA) to investigate structural and elastic properties of YAg, CeAg, HoCu, LaAg, LaZn and LaMg compounds by Sekkal et al. [13]. Palenzona et al. [14] have investigated the phase diagram of Sc–Cd system by differential thermal analysis, metallographic analysis, X-ray diffraction and electron microscopy. Ytterbium compounds/alloys are of special interest because, in many of its compounds, ytterbium is divalent; and in a few compounds it is trivalent. Nipper et al. [15] have found the Yb-In phase diagram by using X-ray diffraction study, differential thermal and metallographic methods. Ozisik et al. [16] have predicted the vibrational and thermodynamical properties of rare earth diborides in AlB_2-type structure based on density functional theory within generalized gradient approximation.

The effect of high pressure on elastic, thermal and mechanical properties of rare earth intermetallic compound RECd and REHg (RE=Sc, La and Yb), has also been effectively examined using full-potential linearized augmented plane wave method within the framework of density functional theory. The paper is organized as follows: in Section 2, a short description of theoretical approach is given. Section 3 is devoted to the results and discussion, finally, we tend to summarize our conclusions in Section 4.

2. Computational method

The first-principles calculations using full potential linearized augmented plane wave method (FP-LAPW) [17] based on the density functional theory as implemented in the latest WIEN2k package [18] have been performed for RECd and REHg (RE=Sc, La and Yb) compounds. In this method, the basis set is obtained by dividing the unit cell into non-overlapping spheres and an interstitial region. The

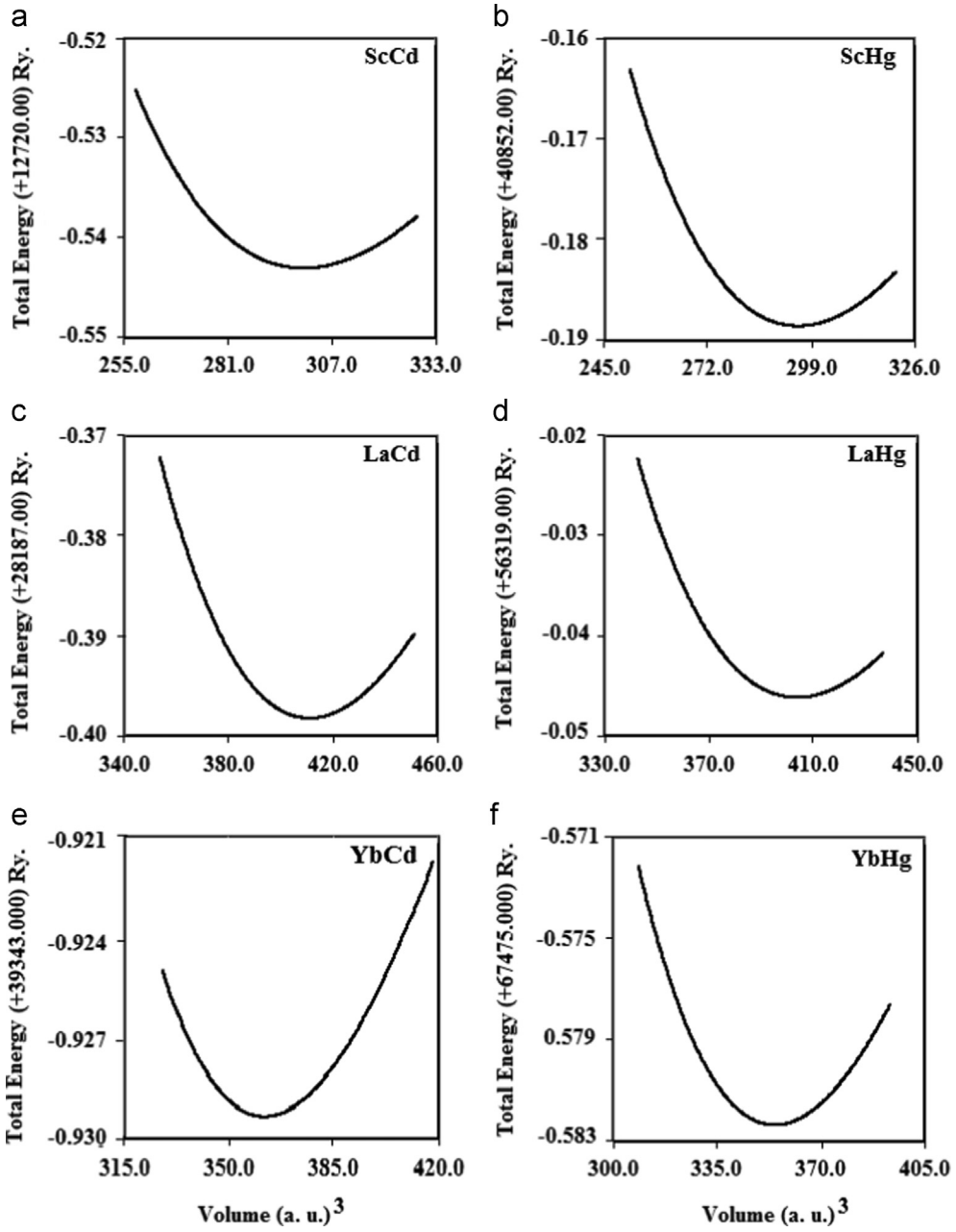

Fig. 1. (a)–(f) Variation of total energy with volume of RECd and REHg compounds in CsCl structure.