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Theoretical prediction of the electronic structure, bonding behavior and elastic moduli of scandium intermetallics

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ABSTRACT

We report the structural, electronic, bonding, elastic and mechanical properties of nine scandium intermetallic compounds, ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Zn, Cd and Hg), using *ab initio* density functional theory with the generalized gradient approximation for exchange and correlation potentials. The calculated structural parameters, such as the lattice constant (a_0), bulk modulus (B) and its pressure derivative (B_0) and elastic constants, are calculated using the CsCl-(B_2 phase) structure. The electronic and bonding properties of the ScX compounds are quantitatively analyzed using band structures, DOS, Fermi surfaces and contour plots. The mechanical properties and ductile behaviors of these compounds are also predicted based on the calculated elastic constants.

1. Introduction

Since the discovery of a new class of fully ordered, stoichiometric, binary, ductile rare-earth/transition-metal intermetallic compounds with body-centered B_2 structures by Gischneidner et al. [1], there has been significant interest among physicists and materials scientists to study their properties in detail, such as their ductility, high tensile strength and high corrosion resistance. Recently, Sun et al. [2] reported a stability map for ductility in ideal B_2 compounds, which is based on dimensionless ratios of elastic constants and defect energies. In general, the ductile nature of AB intermetallics with the B_2 structure has attracted considerable interest because of their superior mechanical properties for practical applications. Scandium forms a series of ordered intermetallic compounds with transition metals (TMs), such as Ru, Co, Rh, Ir, Ni, Pd, Pt, Cu, Au, Ag, Zn, Cd and Hg, and these intermetallics crystallize with the cubic CsCl (B_2) structure [3]. Some of these compounds are of interest for their ductility and high fracture resistance. Various studies on the structure, electronic properties, bonding, specific heat and susceptibility of Sc–TM compounds in the B_2 phase have been reported [4–7].

The electronic properties of B_2-type Sc–TM (TM = Ag, Cu, Pd, Rh and Ru) compounds have been studied both experimentally [3,6] and theoretically [8–11]. The theoretical band structure studies [8] of these compounds show that for Sc–TM (TM = Ag, Cu and Pd), the major contribution to the density of states at the Fermi level is the '*d*' states of Sc, whereas the major contribution is from both the Sc-3*d* and TM-4*d* states for other intermetallics (TM = Rh and Ru). Kubler et al. also reported a detailed study on the electronic structures of ScRu, ScRh, ScPd and ScAg intermetallics with the CsCl structure type using self-consistent calculations [9]. The elastic constants and various other mechanical properties of ScX (X = Ag, Cu, Pd, Ru and Rh) compounds were determined using the full potential linearized augmented plane wave method (FP-LAPW) method [10]. Compared to the other Sc–TM compounds studied by these authors, ScRh was found to be stronger and stiffer and ScRu was found to be more ductile. Inadelli et al. investigated binary intermetallic compounds of Sc with transition metals [12].

Although extensive studies on the electronic properties of Sc–TM (TM = Rh, Ir, Pd and Pt) have already been carried out, to the best of our knowledge, no data are available for Sc–TM (TM = Co, Ni, Zn, Cd and Hg). In addition, very few studies on the elastic properties of the above Sc–TM compounds are available in the literature. This fact

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motivated us to investigate the electronic, elastic and thermal properties of these intermetallic compounds. To obtain a proper understanding of the electronic structures, particularly the bonding nature, we have also studied the Fermi surface topology and charge density plots of these compounds. In Section 2, we briefly outline the computation method, and in Section 3, various results are presented. A brief conclusion is drawn in Section 4.

2. Calculation methods

The present calculations have been performed using the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [13], which is based on density functional theory (DFT). The generalized gradient approximation (GGA) in the scheme of Perdew, Burke and Ernzerhof (PBE) is used for the exchange and correlation effects [14]. To achieve convergence, we expand the basis function up to $R_{MT} \times K_{max} = 7$, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} provides the magnitude of the largest k vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is $l_{max} = 10$, while the charge density is Fourier expanded up to $G_{max} = 12$. The self-consistent calculations are considered converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 k points and the tetrahedral method [15] have been employed for the Brillouin zone integration. The total energies are fit to the Birch [16] equation of state to obtain the ground-state properties.

Determining the elastic moduli requires knowledge of the derivative of the energy as a function of the lattice strain. It is well known that a cubic system has only three independent elastic constants, namely C_{11}, C_{12} and C_{44}. Hence, a set of three equations is needed to determine all the constants. The first equation consists of calculating the bulk modulus (B), which is related to the elastic constants as follows:

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{1}$$

The second step involves the volume-conservative tetragonal strain, which is given by the following tensor:

$$\begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \left(1/(1+\delta)^2\right) - 1 \end{bmatrix} \tag{2}$$

where $\delta = (1+e)^{-1/3} - 1$ with e as a strain tensor. The application of this strain has an effect on the total energy from its unstrained value as follows:

$$E(\delta) = E(0) + 3(C_{11} - C_{12}) + V_0\delta^2 + O\left(\delta^3\right) \tag{3}$$

where V_0 is the volume of the unit cell.

Finally, for the last type of deformation, we use the volume-conserving rhombohedral strain tensor given by:

$$\frac{\delta}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \tag{4}$$

which transforms the total energy to

$$E(\delta) = E(0) + \frac{1}{6}(C_{11} + 2C_{12} + 4C_{44}) + V_0\delta^2 + O\left(\delta^3\right) \tag{5}$$

The thermal loss mechanisms (temperature dependence) of a material are most suitably described in terms of the Debye temperature (θ_D), which is a fundamental parameter closely related to many physical properties, such as elastic constants, specific heat and melting temperature. One of the standard methods for calculating the Debye temperature is to use the elastic constants because θ_D may be estimated from the average sound velocity v_m by the following equation [17,18]:

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi V_a}\right]^{1/3} v_m \tag{6}$$

where h is Plank's constant, k_B is Boltzmann's constant, V_a is the atomic volume, n is the number of atoms per formula unit, and v_m is average sound velocity. The average sound velocity is approximated from Refs. [17,19]:

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-1/3} \tag{7}$$

where v_t and v_l are the transverse and longitudinal sound velocities, respectively, obtained using the elastic constants as follows:

$$v_l = \sqrt{\frac{\left[C_{11} + \frac{2}{5}(2C_{44} + C_{12} - C_{11})\right]}{\rho}} \tag{8}$$

$$v_t = \sqrt{\frac{\left[C_{44} - \frac{1}{5}(2C_{44} + C_{12} - C_{11})\right]}{\rho}} \tag{9}$$

where C_{11}, C_{12} and C_{44} are second-order elastic constants and ρ is the mass density per unit volume.

3. Results and discussion

3.1. Structural properties

For the ground-state properties of scandium compounds (ScTM, TM = Co, Rh, Ir, Ni, Pd, Pt, Zn, Cd and Hg), the total energies are calculated as a function of volume in the CsCl-type structure (B_2 phase) using the first principles FP-LAPW method. The plots of total energy versus reduced volume (E–V) are shown in Fig. 1(a)–(i). As indicated by the E–V curves, the B_2 phase is mechanically stable under ambient conditions. The calculated total energies are fit to the Birch equation of state [16] to determine the ground-state properties, such as the lattice constants a_0, bulk moduli B and its pressure derivatives B_0'. The ground-state properties of these compounds are presented in Table 1. The calculated lattice parameters are in reasonable agreement with the previously reported results [2,8,9,12]. ScIr possesses the largest bulk modulus, which indicates that this compound is the hardest of all the investigated Sc compounds. The bulk moduli of ScRh, ScPd and ScPt are in good agreement with previously reported results [2,9,10].

3.2. Electronic properties

The non-spin polarized electronic band structures along the high symmetry direction of the ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Zn, Cd and Hg) compounds are presented in Fig. 2. The Fermi level is fixed at the origin. The total and partial densities of states (DOS) for these compounds at ambient pressure are presented in Fig. 3. The overall electronic band structures of all the compounds show only slight changes, which are discussed later. Fig. 2(a)–(c) present the