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Band Structure Calculation of AgCd and AgZn Intermetallics

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Abstract *– The electronic band structure of non magnetic AgCd and AgZn intermetallic compounds, which crystallize in the CsCl-type (B_2 phase) structure was studied by means of the self-consistent tight binding linear muffin tin orbital method at ambient conditions. The total energies are computed as a function of volume and fitted to the Birch equation of state. The ground state properties such as the equilibrium lattice parameter; the bulk modulus and the cohesive properties of these compounds are calculated.*

Keywords*: TB-LMTO; Inter-metallic compounds; Electronic band structure.*

I. Introduction

Intermetallic materials have drawn a considerable interest in last decade for inorganic chemists, physicists and material scientists [1-3]. Recently, the binary intermetallics (AB-type, where 'A' is metal; 'B' is metal/transition metal or rare earth) and alloys [4,5] are recognized because of their significant applications in material design due to their ductile and high tensile strength. These metals are bonded with specific stoichiometries by mixed metallic, covalent and ionic bonding. Both the species in intermetallics are ordinary metals and their chemical, physical, electrical, magnetic and mechanical properties are often superior. Ag-rich -Cd and -Zn intermetallics crystallize in cubic cesium chloride structure (B_2, *Pm3m*, Space Group, *221*). There are number of intermetallics, which have the similar CsCl-type structure, are studied experimentally and theoretically [4-7]. To the best of our knowledge the structural and electronic properties of AgCd and AgZn intemetallics under ambient conditions, have not been extensively studied and those are yet to be explored in details. In this paper we present a first principles tight binding linear muffin tin orbital (TB-LMTO) study to build further confidence in this approach and to provide important crystal chemical information. Theoretical data in this area can usefully supplement experiment in various cases where x-ray diffraction data is not possible. The organization of the paper is prearranged as follows: the methodology that has been used to calculate electronic properties of AgCd and AgZn intermetallics and the first principles computational details are briefly provided in Section 2. The results and discussion on electronic properties are then presented in Section 3 with the concluding remarks of the present work.

II. Method of Calculations

The self consistent non-spin polarized TB-LMTO [8,9] method within the atomic sphere approximation (ASA) [10], was used to calculate total energy, band structure and density of states for AgCd and AgZn intermetallic compounds. These intermetallics crystallize in the B_2 phase, and positioned at Ag: (0, 0, 0) and Cd/Zn: (0.5, 0.5, 0.5). In the present calculation this method does not include empty spheres because these intermetallics belong to CsCl-type close-packed structure. As already mentioned [3], the TB-LMTO is best suited for close-packed structures. For the exchange-correlation potential within the local density approximation (LDA), the parameterization scheme of the van-Barth and Hedin [10] has been used. The Wigner-Seitz sphere radius was chosen in such a way that the sphere boundary potential was minimum and the charge flow between the two atoms was in accordance with the electro-negativity criteria. The **E** and **k** convergence was checked consequently. The tetrahedron method [11] of Brillouin zone integration had been used to calculate the total density of states. The total energy was computed by reducing the volume from 1.00 V_0 to 0.65 V_0, where V_0 is the equilibrium cell volume. The calculated total energy was fitted to Birch equation of state [12] to obtain the pressure volume relation. The pressure was obtained by taking volume derivative of the total energy. The bulk modulus $B = -V_0 \, dP / dV$ was also calculated from P-V relation.

III. Results and discussion

To study structural and electronic properties, the modern *ab-initio* simulation provides a powerful tool with reasonable confidence. Therefore, it is done by

computing the band structure, density of states, bulk modulus and cohesive energy etc. The non spin polarized electronic band structure calculations are carried out to estimate the total energy of the intermetallics by using first principles TB-LMTO method. The total energy is plotted against different compressions and shown in Fig. 1. The minimum of the curves define the equilibrium volume V_0 (or equilibrium separation, r_0), which is found to be Å^3 for AgCd and the corresponding lattice parameter a, Å. Similarly, AgZn intermetallic estimates equilibrium volume at Å^3 and the corresponding lattice parameter value Å and are tabulated in Table-I. Due to unavailability of the experimental data, we could not compare our results with those of the experiment data.

TABLE I

Calculated properties of lattice parameter, a , bulk modulus, B_0, first order derivative, B'_0, and total energy, E_{tot} for AgCd and AZn intermetallics

Solid	a (Å)	B_0 (GPa)	B'_0 (Å)	E_{tot} (Ry.)
AgCd	3.25	12.71	3.81	-21805.
Present	3.33[a]	-	-	-
Others'.				
AgZn	3.07	14.11	3.60	-14211.
Present	3.16 [a]	-	-	-
Others				

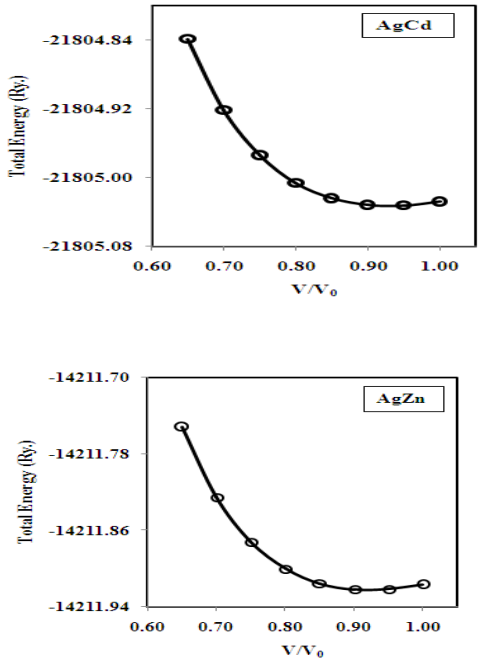

Fig. 1 Variation of total energy with relative volume for AlRE (RE=Ho, Er, Tm and Yb) intermetallics.

The self consistent band structures along the high symmetry directions for these intermetallics are obtained and shown in Fig.2. On the whole band profile is found to be almost same. It is seen from the Fig. 2 that lowest lying band in these compounds is mainly due to 'd' like states (AgCd: Ag-d near -5 eV; Cd-d near -10 eV, AgZn: Ag-d near -5 eV; Zn-d near -8 eV) relative to Fermi level. The crossover of bands at Fermi level is mainly due to Ag 'p' like states, which hybridized with the Cd/Zn 'p' like states and shows a metallic nature of compounds.

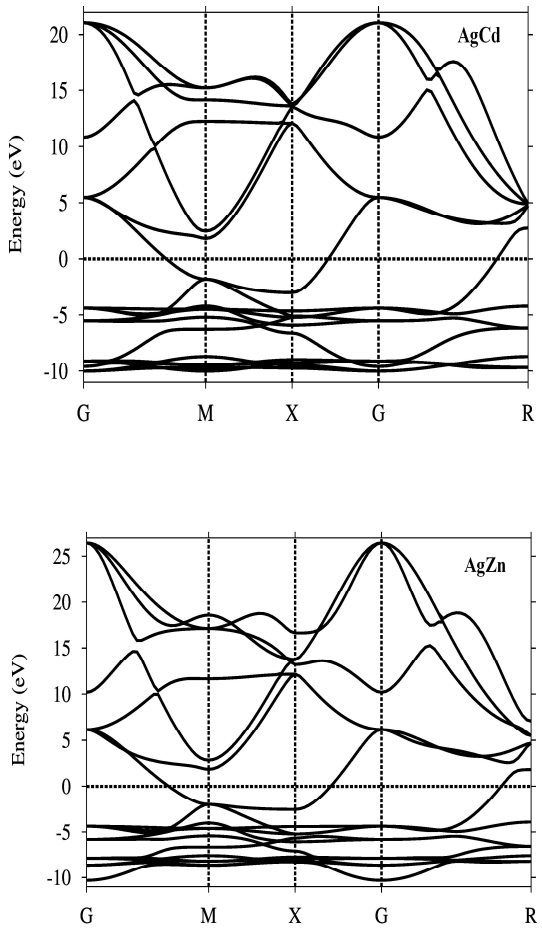

Fig. 2 Band structure along high symmetry direction of (i) AgCd (ii) AgZn intermetallics.

The density of states (DOS) plot provides an even comprehensible picture of the elemental contributions to the electronic structure of Ag-intermetallics. In Fig. 3 we show typical DOS of AlRE intermetallics under ambient conditions. In Fig 3 a peak at – 5eV corresponds to Ag 'd' like states, while another peak at -10 eV /-8 eV is mainly due to Cd/Zn 'd' like states. At Fermi level metallic nature can be understood by crossover of p like states of Ag and Cd/Zn.

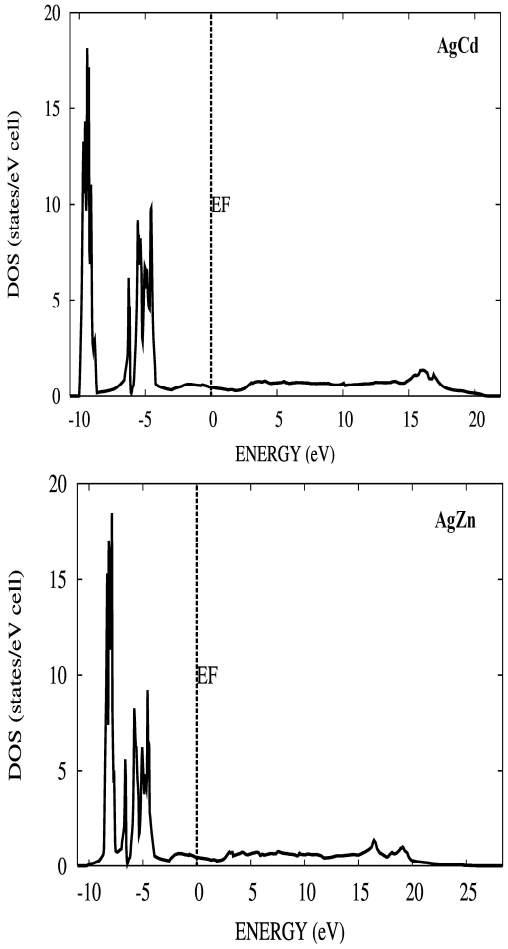

Fig. 3 Total density of states at Fermi level of (i) AgCd (ii) AgZn intermetallics.

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Author's Profile

Ms. Neetu Paliwal *was born in 1976 in India. She was graduated in 1999 from Barkatullah University, Bhopal, India. She got her Master of Science and Master of Philosophy in Physics in 2001 and 2007, respectively from Barkatullah University, Bhopal, India. She is pursuing Ph. D. in Physics from AISECT University, Bhopal, India. Presently, she is Heading Department of Physics in the same University. She attended several National and International conferences. Her interest is in Intermetallics. She is looking all the electronic and thermal properties of some binary intermetallics.*

Dr. Vipul Srivastava *was born in Sheopur Kalan, India in 1973. He got post graduated (Applied Physics) in 1997 at Barkatullah University Bhopal, India. Vipul was awarded Ph.D degree in Physics in 2005 from Barkatullah University Bhopal. In 2006 he was awarded as a Young Scientist by the Department of Science & Technology, New Delhi and joined Department of Physics, Barkatullah University, Bhopal, India. In 2008, he joined Department of Physics, NRI Institute of Reasearch and Technolgy, Bhopal , India as Associate Professor and still serving in the same institute. His research interest is investigation of Structural Phase Transition and Electronic, Mechanical properties of some materials under normal as well as high pressure.Vipul has predicted various properties in Rare Earth and Intermetalic compounds. During his research career, he was invited by the University of California, Berkeley, USA in 2004 to deliver a lecture on high pressure study. In 2004, he got training in Summer School at Abdus Salam International Center for Theoretical Physics (ICTP), Trieste, Italy. Recently, he was invited by National University of Singapore (NUS), Material Research Society in 2011. Vipul has been a reviewer of various international journals. He has 35 publications in different international journals and 25 in proceedings. Dr. Vipul is an Editor-in-Chief of International Journal of Emerging Interdisciplinary Trends in Engineering. Vipul has been a peer reviewer for international journals like Physica B Condenced Matter Physics, European journal of modern physics.*