

Investigation on Mechanical Properties of Mn_3Sb Intermetallic Compound

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In this work, *ab initio* calculation has been performed to investigate the structural, elastic and mechanical properties of Mn_3Sb intermetallic compound, based on density functional theory plane-wave pseudo potential method within local density approximation and generalized gradient approximation. The calculated structural parameter in both approximations of Mn_3Sb compound is consistent with the experimental data. The elastic constants were determined from a linear fit of the calculated stress-strain function according to the Hooke law. From the elastic constants, the bulk modulus B , shear modulus G , the Young modulus E , the Poisson ratio σ , anisotropy factor A and the ratio B/G for Mn_3Sb compound are obtained. This is the first quantitative theoretical prediction of these properties.

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1. Introduction

Intermetallics are known to be of great technological importance and high scientific interest, because they are used in a wide range of industries [1]. Extensive investigations on the preparation of intermetallic compounds have been made in Mn-Sb binary system. There were found two intermediate phases, Mn_2Sb and MnSb in the equilibrium phase diagram [2]. In recent years, a new intermetallic compound, Mn_3Sb , has been successfully synthesized under high pressure and temperature condition [3, 4]. In the literature only, the structural and magnetic properties of Mn_3Sb are investigated experimentally [3, 5]. To the best of our knowledge, it is the first theoretical study of the intermetallic compound Mn_3Sb . Thus, in this work we have carried out a theoretical investigation on the structural, elastic and mechanical properties of Mn_3Sb , in order to provide a sounder basis for further experimental and theoretical studies. The rest of this paper is organized as follows: the computational method is described in Sect. 2, the numerical results and discussions are given in Sect. 3, and finally a conclusion is presented in Sect. 4.

2. Computational method

Ab initio calculations are performed with the plane-wave pseudopotential (PW-PP) total energy method implemented with the Cambridge Serial Total Energy Package (CASTEP) simulation program [6]. This is based on the density functional theory (DFT) [7, 8].

We have used two approximations for electronic exchange-correlation potential energy: the local density approximation (LDA) developed by Ceperley and Adler and parametrized by Perdew and Zunger [9, 10], as well

as the generalized gradient approximation (GGA), with the functional of Wu and Cohen, known as WC [11]. The Coulomb potential energy caused by electron-ion interaction is described using the Vanderbilt-type ultrasoft scheme [12], in which the orbitals of Mn ($3d^54s^2$), Sb ($4d^{10}5s^25p^3$) are treated as valence electrons. The cut-off energy for the plane-wave expansion was chosen at 280 eV and the Brillouin zone sampling was carried out using the $8 \times 8 \times 8$ set of the Monkhorst-Pack mesh [13]. The structural parameter (a) of Mn_3Sb was determined using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization technique [14]. This method usually provides the fast way of finding the lowest energy structure.

In the structural optimization process, the energy change, maximum force, maximum stress and maximum displacement are set as 1.0×10^{-5} eV/atom, 0.03 eV/Å, 0.05 GPa, and 0.001 Å, respectively.

The elastic constants were determined from first-principles calculations by applying a given homogeneous strain (deformation) with a finite value and calculating the resulting stress. The total energy is converged to 2.0×10^{-6} eV/atom in the self-consistent calculation.

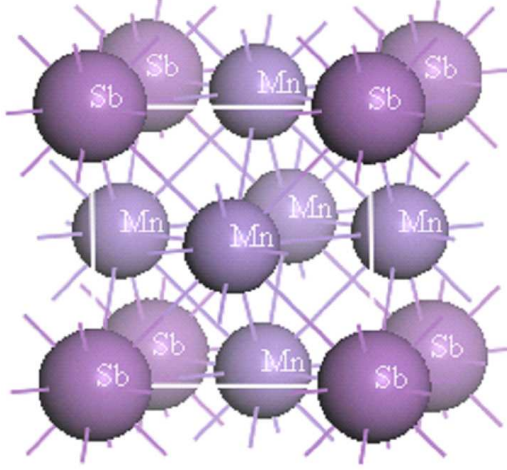
3. Results and discussion

3.1. Structural properties

The Mn_3Sb compound crystallizes into a cubic structure with the space group $Pm-3m$ (221), namely the $L1_2$ -type structure. The structure was refined by the Rietveld analysis of the powder X-ray diffraction data and the equilibrium lattice parameter was determined to be $a = 4.0017$ Å [3]. Manganese (Mn) atoms are located at the face-centered positions and antimony (Sb) atoms at the corners of the cubic unit cell. The unit cell structural model of the Mn_3Sb compound is built according to the experimental data [3], as shown in Fig. 1.

The crystal structure was optimized at first. The obtained results of calculated lattice parameter a of Mn_3Sb

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Fig. 1. Crystal structure of Mn_3Sb .

intermetallic compound using the PW-PP method within both the LDA and the GGA-WC approximations are given in Table I, together with experimental data for comparison. From the present results in Table I, one can see that the calculated lattice constant is underestimated by LDA and GGA-WC approximations. It is 6.86% smaller than the experimental value using LDA and it is only 5.11% smaller than the experimental value using GGA-WC. We can say that our calculated equilibrium lattice parameter agrees well with the experimental data in both approximations. The interatomic distances are also estimated and the results are listed in Table I, together with experimental data. It can be seen from Table I that the calculated bond lengths in Mn_3Sb compound are consistent with the experimental data. They deviate from experimental ones by 7.36% and 5.38% in LDA and GGA approximations, respectively.

TABLE I

Lattice parameter (a) and interatomic distances in Mn_3Sb .

	Present work		Experiment
	LDA	GGA	
a [Å]	3.7271	3.7972	4.0017 ^a 3.9980 ^b
Mn–Mn [Å]	2.6355	2.6850	2.8296 ^a
Mn–Sb [Å]	2.6355	2.6850	2.8296 ^a

^aRef. [3], ^bRef. [4].

3.2. Elastic and mechanical properties

The elasticity of a cubic crystal is specified by the three independent elastic constants C_{11} , C_{12} and C_{44} . In this work, the calculated elastic constants of Mn_3Sb compound at zero pressure and temperature are presented in Table II.

For a cubic crystal, the obtained elastic constants meet the requirements of mechanical stability criteria:

TABLE II

Calculated values of the elastic constants C_{ij} [GPa], bulk modulus B [GPa], shear modulus G [GPa], the Young modulus E [GPa], the Poisson ratio σ , anisotropy factor A and B/G of Mn_3Sb compound. There is no experimental or theoretical results for these parameters.

	C_{11}	C_{12}	C_{44}	B	G	E	σ	A	B/G
LDA	313.89	174.25	147.99	220.79	109.47	281.83	0.29	2.12	2.02
GGA	280.87	142.52	129.75	188.64	100.81	256.70	0.27	1.88	1.87

$C_{11} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$ and $C_{11} > B > C_{12}$. From Table II, one can see that the elastic constants of Mn_3Sb compound satisfy all of these conditions, suggesting that the structure of Mn_3Sb is mechanically stable. The elastic constants values calculated using the LDA approximation are slightly higher than those obtained with the GGA-WC approximation.

To the best of our knowledge, there are no experimental and other theoretical data in literature for the elastic constants (C_{ij}) of Mn_3Sb for comparison, so we consider the present results as prediction study which still awaits an experimental confirmation. The most important parameters for estimating mechanical properties of materials such as bulk modulus (B), shear modulus (G), the Young modulus (E) and the Poisson ratio (σ) are obtained from results of the calculated single-crystal elastic constants C_{ij} using the Voigt–Reuss–Hill (VRH) averaging scheme [15]. The VRH approximation gives the effective values of the bulk and shear moduli. For the cubic system, the Voigt bounds [16] of the bulk modulus B_V and shear modulus G_V are given by the relations

$$B_V = \frac{(C_{11} + 2C_{12})}{3} \quad (1)$$

and

$$G_V = \frac{(C_{11} - C_{12} + 3C_{44})}{5}. \quad (2)$$

The Reuss bounds [17] of the bulk and shear moduli are given by the relations

$$B_R = B_V \quad (3)$$

and

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}. \quad (4)$$

Finally, the bulk modulus B and shear modulus G , based on the Hill approximation [15] are arithmetic average of the Voigt and Reuss elastic moduli, and they are expressed as following:

$$B = \frac{1}{2}(B_V + B_R) \quad (5)$$

and

$$G = \frac{1}{2}(G_V + G_R). \quad (6)$$

the Young modulus (E) and the Poisson ratio (σ) can be calculated by using the Hill elastic moduli B and G , which are given as

$$E = \frac{9BG}{3B + G}, \quad (7)$$

$$\sigma = \frac{3B - 2G}{2(3B + G)}. \quad (8)$$

The calculated results for these moduli and the Poisson ratio for the Mn₃Sb compound are listed in Table II. The bulk modulus is usually assumed to be a measure of resistance to volume change by applied pressure. From Table II, it can be seen that the value of the bulk modulus of Mn₃Sb compound is larger, indicating that it has a strong resistance to volume change by applied pressure. The two constants E and G are all that is needed to fully characterize the stiffness of an isotropic material. The present calculated results of these moduli demonstrate that the Mn₃Sb compound is stiff. The Poisson ratio (σ) defined as the ratio of transverse strain to the longitudinal strain is used to reflect the stability of the material against shear and provides information about the nature of the bonding forces. It takes the value: $-1 < \sigma < \frac{1}{2}$. No real material is known to have a negative value of σ . Therefore this inequality can be replaced with $0 < \sigma < \frac{1}{2}$. The low value of the Poisson ratio indicates a large compression of volume and when $\sigma = 0.5$ no volume change occurs. Bigger the Poisson ratios better the plasticity. The present calculated result of the Poisson ratio shows that the Mn₃Sb intermetallic compound is of good plasticity.

The Zener anisotropy factor (A) is a measure of the degree of anisotropy in solid [18]. It takes the value of 1 for an isotropic material. It provides a measure of the degree of elastic anisotropy, when the A values are smaller or greater than unity. The Zener anisotropy factor (A) of Mn₃Sb compound is calculated by the following equation:

$$A = \frac{2C_{44}}{C_{11} - C_{12}}. \quad (9)$$

As shown in Table I, the calculated Zener anisotropy factor A is larger than 1 for both approximations LDA and GGA, which indicates that the Mn₃Sb compound is elastically anisotropic material.

The ratio B/G is a simple relationship related to brittle or ductile behaviour of materials. It has been proposed by Pugh [19]. A high B/G ratio is associated with ductility, whereas a low value corresponds to the brittleness. The critical value separating ductile and brittle material is 1.75. The calculated results are listed in Table I. In this work, the obtained results of both approximations LDA and GGA indicate that Mn₃Sb compound can be classified as ductile material at zero pressure. Another parameter indicating the brittleness or ductility of the material is the Cauchy relation defined as: $C_P = C_{12} - C_{44}$. The material is expected to be ductile, if the value of this expression is positive, on the other hand, if its value is negative, the material is brittle [20]. At zero pressure, we found 26.26 GPa and 12.77 GPa for the Cauchy pressure within both the LDA and the GGA approximations, respectively. From these values and according to above criterion, the studied compound is ductile. Thus, the ductile nature of Mn₃Sb compound can be related to a metallic character in its bonds.

4. Conclusion

In the present theoretical study, the structural, elastic and mechanical properties of Mn₃Sb intermetallic compound have been investigated by means of the DFT within LDA and GGA approximations. Our results for the optimized lattice parameter (a) are in good agreement with the available experimental data. The elastic constants C_{ij} , and related polycrystalline mechanical parameters such as bulk modulus B , shear modulus G , the Young modulus E and the Poisson coefficient σ are calculated. The Mn₃Sb compound is mechanically stable according to the elastic stability criteria, while there is no experimental results of elastic moduli for comparison. The Zener factor A , the B/G ratio and Cauchy pressure ($C_{12} - C_{44}$) are also estimated. The calculated Zener factor indicates that Mn₃Sb compound is elastically anisotropic. The values of the ratio B/G and Cauchy pressure show a ductile manner for the Mn₃Sb compound.

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