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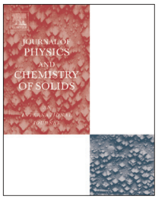

Electronic structure, phase stability, and vibrational properties of Ir-based intermetallic compound IrX (X=Al, Sc, and Ga)

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ABSTRACT

The phase stability and mechanical properties of *B2* type IrX (X=Al, Sc and Ga) compounds are investigated. Self-consistenttotal-energy calculations in the framework of density functional theory using the Generalized Gradient Approximation (GGA) to determine the equations of state and the elastic constants of IrX (X=Al, Sc, and Ga) in the B2 phase have been performed. The calculations predicted the equilibrium lattice constants, which are about 1% greater than experiments for IrAl, 1.81% for IrGa, and 0.71% for IrSc compound. IrAl is shown to be the least compressible, and it is followed by IrGa and the IrSc compound. The phase stability of the studied compounds is checked. The brittleness and ductility properties of IrX (X=Al, Sc, and Ga) are determined by Poisson's ratio σ criterion and Pugh's criterion. IrGa compound is a ductile material; however, IrAl and IrSc show brittleness. The band structure and density of states (DOS), and phonon dispersion curves have been obtained and analyzed. The position of the Fermi level and the contribution of d electrons to the density of states near E_F is studied and discussed in detail. We also used the phonon density of states and quasiharmonic approximation to calculate and predict some thermodynamic properties such as constant-volume specific heat capacity of the B2 phase of IrX (X=Al, Sc and Ga) compounds.

1. Introduction

The search for new high-temperature materials in oxidizing environments for structural applications and coatings has attracted considerable interest. Iridium-based alloys have been selected as the most promising protective coating materials at ultrahigh temperatures [1–4]. The IrAl compound is proposed as a smart oxidation-resistant coating that can form an aluminum layer as a protective coating on the iridium layer by oxidation [5]. The attractive characteristics of Iridium include high melting point (2739 °K), high elastic moduli, and relatively low oxidation rates compared with other high-melting metals. However, it forms gaseous oxides of IrO_3 and IrO_2 instead of a protective oxide scale in high-temperature oxidizing environments [5–8].

To improve the oxidation resistance and suppress the formation of Ir oxides, alloying with Al has been evaluated. Recently, Ir-based alloys have attracted extensive interest for potential high-temperature structural applications [9,10]. Previous studies have demonstrated that binary alloys in Ir–Al or Ir–Hf systems could form external oxide layers if the concentration of Al or Hf is large enough. The formation of a continuous external layer of $A1_2O_3$ [11] or HfO_2 could prevent the formation of gaseous iridium oxides, and oxidation resistance is improved to a great extent [12]. IrAl was prepared by quenching a melt of the same stoichiometry. It was shown that this compound has a cubic CsCl structure with a cell constant of 2.977 Å [13]. Later on IrAl was prepared by reducing Al_2O_3 in the presence of Iridium at 1600 °C, and a lattice parameter of 2.983 Å was found [14]. Axler and Roof produced the IrAl crystal with a cubic CsCl structure by a molten metal flux containing Th, Ir, and Cu. They measured a lattice constant of 2.9867 Å [15]. The phase diagram of Al–Ir system has been presented [10,16–19] and studied and the existence of Al_9Ir_2, Al_3Ir, $Al_{2.7}Ir$, $Al_{13}Ir_4$ and AlIr has been confirmed. The peritectic temperatures were determined for all the compounds, and a melting temperature of about 2120 °C was found for AlIr [16]. Lee and Worrell prepared Ir–Al alloys of several different compositions. They found that the samples whose aluminum content varied from 40 to 74 at% were either single-orbinary-phase alloys of Ir,

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IrAl, IrAl$_{2.5}$ and IrAl$_{3.}$ A melting temperature of 1600–1650 °C for IrAl$_{2.5}$ and for IrAl of above 1800 °C is suggested [20]. A thermodynamic modeling of the binary Al–Ir system was performed using a combined first-principle and CALPHAD approach. The formation enthalpies of all six stable intermetallic compounds in the Al–Ir system were obtained [21]. The thermodynamic assessment of the Al–Ir binary system was performed using the CALPHAD technique. The thermodynamic quantities, such as the phase equilibria, invariant reactions, and formation enthalpies of the intermetallic phases, were calculated and agree well with experimental data [22]. Binding energy for the nine 4d transition metal aluminides (TmAl) with regard to twelve different AB-structure types has been computed using the full-potential linear muffin-tin orbitals (FP-LMTO) method within local-density-functional approximation (LDA) [23]. The high-temperature compression strength, the creep properties and deformation mechanisms of the Ir-based system with an fcc and a B2 two-phase structure at 1773 °K were discussed [11]. The IrAl phase with a B2 structure was identified by Fleischer as having good high-temperature strength and reasonable toughness at ambient temperature [24]. The significantly higher melting temperature of IrAl is expected to lead to the realization of a useful high- temperature structural material [9,25]. The effect of Co addition to IrAl on oxidation behavior was studied, and Co addition was expected to enhance B2- phase stability. It is concluded that the oxidation resistance of IrAl alloys was dramatically improved by Co addition [4]. Thus, it is found that the addition of Ni improves the ductility of IrAl [5]. The analysis for the electronic structure of intermetallic compounds ScB (B=Cu. Ag, Pd, Rh, Ir, and Ru) is given in terms of local susceptibilities, as well as in terms of a two-band model. Accordingly, ScIr belong to group III; the d spin and orbital contributions originate from A and B sites. The d spin contributions are much smaller than those of groups I or II [26]. This is consistent with high-resolution ultraviolet photoelectron spectra for Sc, ScAg, ScPd, ScIr, and ScRu [27] as well as band-structure calculations [28] which found that there are d contributions to the density of states near E_F originating from the Sc site in ScAg and ScPd, possibly from both sites in Sclr and from the Ru site in ScRu. With a fully automated high-temperature calorimeter the enthalpy of formation of the Ir–Ga liquid system was determined between $1060\ \text{K} < \text{T} < 1471\ \text{K}$, in the molar fraction range $0 < x < 0.54$ [29].

Despite the promising performances of Ir-based binary compounds in structural and coating application fields, and the intensive investigations on IrAl to improve its mechanical properties such as toughness, ductility, and high-temperature strength, as well as oxidation resistance, only limited information is available for the structural, electronic, and vibrational properties of IrX (X=Al, Sc and Ga) compounds. This article is organized as follows. Section II is devoted to the description of our calculational methods. In Section 3, we discuss the results of our calculations with regard to the structural, electronic, and vibrational properties of IrX (X=Al, Sc, and Ga) compounds, including the checking of their stability. The ductility and brittleness of these intermetallics is examined. A summary is provided in Section 4.

2. Structure and method of calculation

Intermetallics are compounds that are not mixtures and whose crystal structures are different from those of the constituent metals. The crystal structure of an intermetallic compound is determined by the strength and character of bonding in the crystal, which depends on the particular electronic configuration and the relative atomic sizes. Many intermetallics with the composition AB crystallize in the *B2* (CsCl) structure [30].

The ground-state energies and electronic structures were calculated using density functional theory (DFT) [31] within the generalized-gradient approximation (GGA) [32]. The quantum-Espresso code that incorporates the self-consistent ultrasoft pseudopotential method was used [33]. The electronic configurations used were $3s^2 3p^1$ for aluminum, $3d^1 4s^2$ for scandium, $4s^2 4p^1$ for gallium, $5d^7 6s^2$ for Iridium.

A plane-wave basis set with an energy cut-off of 40 Ry was applied. The electronic charge density was evaluated for an approximate kinetic energy cut-off of 400 Ry. The **k**-point meshes for Brillouin zone sampling were constructed using the Monkhorst-Pack scheme [34]; the (10 × 10 × 10) **k**-points mesh was used for all calculations. The phonon frequencies were calculated. The lattice-dynamical properties were calculated using the density functional linear response method [35]. The ground state of each compound was found by minimizing the total energy as a function of the lattice parameters. Elastic constants were obtained from the slopes of the acoustic branches in the phonon dispersion curves [36]. The sound velocities correspond to the small-wavelength behavior of the acoustic phonons. These velocities are associated with C_{11}, C_{44} and C_{12} as they are described in [30,36]. Once the single crystal elastic constants are computed, the related polycrystalline properties such as Young's modulus (E), Shear modulus (G) are derived using the following standard relations:

$$G = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{1}$$

Young's modulus (E) of a material is a key parameter for mechanical engineering design

$$E = \frac{9BG}{3B + G} \tag{2}$$

Another crucial elastic moduli considered as having a significant implication in engineering science is the elastic anisotropy of crystals A. For a completely isotropic material $A=1$, values smaller or greater than unity measure the degree of elastic anisotropy. The anisotropy factor A is given by

$$A = \frac{2C_{44}}{(C_{11} - C_{12})} \tag{3}$$

Poisson's ratio is also of interest, and it is defined as the ratio of the lateral contraction to the elongation

$$\sigma = \frac{1}{2}\left(1 - \frac{E}{3B}\right) \tag{4}$$

In the quasiharmanic approximation (QHA), the constant-volume specific heat capacity C_v, internal energy E, phonon free energy F and entropy S are given by

$$C_v = 3nNk_B \int_0^{\omega_{max}} \left(\frac{\hbar\omega}{2k_BT}\right)^2 \operatorname{csch}^2\left(\frac{\hbar\omega}{2k_BT}\right) g(\omega)d\omega \tag{5}$$

$$\Delta F = 3nNk_BT \int_0^{\omega_{max}} \ln\left\{2 \sinh \frac{\hbar\omega}{2k_BT}\right\} g(\omega)d\omega \tag{6}$$

$$\Delta E = 3nN\frac{\hbar}{2} \int_0^{\omega_{max}} \omega \coth\left(\frac{\hbar\omega}{2k_BT}\right) g(\omega)d\omega \tag{7}$$

$$S = 3nNk_B \int_0^{\omega_{max}} \left[\frac{\hbar\omega}{2k_BT} \coth \frac{\hbar\omega}{2k_BT} - \ln\left\{2 \sinh \frac{\hbar\omega}{2k_BT}\right\}\right] g(\omega)d\omega \tag{8}$$

where n is the number of atoms per unit cell, N is the number of unit cell, ω is the phonon frequency, $g(\omega)$ is the phonon density of states, $\hbar$ is Planck's constant, k_B is Boltzmann's constant, and T is temperature.

3. Results and discussion

3.1. Equilibrium lattice determination, elastic properties and mechanical stability

As a starting point to understand the physical properties of Ir-based alloys and to improve their mechanical properties, such as toughness, ductility, and high-temperature strength, as well as oxidation resistance, the structural, electronic, and vibrational properties of IrX (X=Al, Sc and Ga) compounds have been studied. It has been found that the IrX (X=Al, Sc, and Ga) compounds were stable in the B2 phase [13–15]. The lattice constants and bulk modulus have been optimized by minimizing the total energy with regards to volume using the equation of state (EOS) by Murnaghan [37]. In Table 1, we summarize our calculated equilibrium lattice constants of IrX (X=Al, Sc, and Ga) compounds compared with the available experimental and theoretical data [13–15,17,25,28,38]. Our values of the lattice parameter agree well with the experiment. The calculations predicted the equilibrium lattice constants which are about 1% greater than experiments for IrAl, 1.81% for IrGa, and 0.71% for IrSc. It is clearly seen that the lattice constant increases as we progress from IrAl to IrGa to IrSc. On the other hand, the bulk modulus decreases as we move from IrAl to IrGa to IrSc. The bulk modulus decreases by 5% when we replace Al by Ga, and by 26% when we substitute Sc for Al. We mention that the bulk modulus of IrAl is the largest one of about 229.3 GPa, and as a result, it is predicted to be the hardest in the studied series. IrAl is shown to be the least compressible, followed by IrGa and then the IrSc compound. The calculated bulk modulus decreases from IrAl to IrSc, suggesting that the compressibility increases from IrAl to IrSc. We note that the Ir atoms are the same in the three compounds, the size of X atoms is different.The different size of the X atoms could be responsible for the lattice constant increasing from IrAl to IrSc.

The calculated elastic constant C_{ij} can be used to check the phase stability of the studied compounds, and to provide an estimation of the strength and, indirectly, the melting temperature [39]. To obtain the elastic constants of these compounds with a cubic structure, we have used the method described in [36]. Our calculated elastic constants are presented in Table 1. To the best of our knowledge, no experimental or theoretical values for the elastic constants of these compounds have appeared in the literature; so, our results for the B2 phase can serve as a reference for future investigations.

The well-known Born stability criteria are a set of conditions on the elastic constants (C_{ij}) that are related to the second-order change in the internal energy of a crystal under deformation. The requirement of the mechanical stability in a cubic crystal leads to the following restrictions on the elastic constants [40]:

$$C_{44} > 0, (C_{11} - C_{12})/2 > 0 \textit{ and } B = (C_{11} + 2C_{12})/3 > 0.$$

From Table 1, one can see that the calculated elastic constants of cubic IrX (X=Al, Sc and Ga) obey these mechanical stability conditions, including the fact that B should be larger than C_{12} and smaller than C_{11}. So as a conclusion all the compounds are stable in the B2 phase.

In the present work, brittleness and ductility properties of IrX (X=Al, Sc, and Ga) compounds have been investigated by calculating the B/G. The critical value that separates brittleness and ductility is around 1.75. If B/G value is smaller than 1.75, the material behaves in a brittle manner; otherwise, the material is a ductile compound [41]. According to this empirical law, the IrGa compound is a ductile material; however, IrAl and IrSc show brittleness. According to Frantsevich et al. [42], Poisson's ratio can also be used to distinguish the brittleness from ductility in metal, and intermetallic materials. Metals having Poisson's ratios around 1/3 are ductile, whereas metals having Poisson's ratios less than 1/3 are inferred as being brittle. On the basis of Poisson's ratio shown in Table 2, the brittleness and ductility properties of IrX (X=Al, Sc, and Ga) determined by Poisson's ratio σ criterion are in good agreement with the results estimated by the B/G ratio, The derived quantities from the elastic constants are given in Table 2, and the related mechanical behavior of the materials under study is explained here. From our reported values in Table 2, we can see that Young's modulus of IrX (X=Al, Sc and Ga) compounds range from 268 to 423 GPa, and the anisotropy factor (A) increases the value of 2.3 to approximately 2.53. This enables us to conclude that the IrAl is the stiffest material, and all the compounds are strongly anisotropic elastically.

3.2. Electronic and vibrational properties

The band structure of IrX (X=Al, Sc, and Ga) compounds along the high symmetry directions in the Brillouin zone is shown in Fig. 1. The calculated total and the projected density of states (DOS) are shown in Fig. 2. There is no band gap in the DOS at the Fermi level (E_F), and, hence, IrX is metallic. The bands near the Fermi level are mainly contributed by Ir-d-orbitals for IrAl and IrGa and by Ir-d and Sc-d orbitals for IrSc compound, because the d shell at the Sc site is no longer filled. This is in good agreement with previously reported works [26,27] which show based on band-structure calculations that there are d contributions to the density of states near E_F originating from both sites Sc and Ir in

Table 1
Calculated lattice constant a (in Å), cohesive energy ($Ecoh$) per unit cell in eV,bulk modulus B (in GPa) and elastic constants C_{ij} (GPa) for IrX (X=Al, Sc and Ga) compounds, compared with the available experimental and theoretical data.

Compounds	**References**	**a(Å)**	***Ecoh*(eV/cell)**	***B*(GPa)**	**C_{11}(GPa)**	**C_{12}(GPa)**	**C_{44}(GPa)**
IrAl	This work	3.012	14.92	229.3	394.63	196.28	229.86
	VASP [21]	3.020					
	Exp. [13]	2.980					
	Exp. [15]	2.9867					
	Exp. [14]	2.983					
	Exp. [25]	2.986					
IrSc	This work	3.230	15.91	168.4	279.82	147.13	152.745
	Exp. [28]	3.206					
IrGa	This work	3.059	12.78	216.5	316.03	207.79	137.18
	Exp. [38]	3.004					
	Exp. [38]	3.010					

Table 2
Calculated shear modulus *G* (GPa), *B*/*G*, Young's modulus *E* (GPa), Poisson's ratio *σ*, anisotropy factor *A* for IrX (X=Al, Sc and Ga) compounds.

Compounds	*G*	*B/G*	*E*	*σ*	*A*
IrAl	177.586	1.291	423.443	0.192	2.317
IrSc	118.185	1.424	287.336	0.215	2.302
IrGa	103.956	2.082	268.838	0.293	2.534

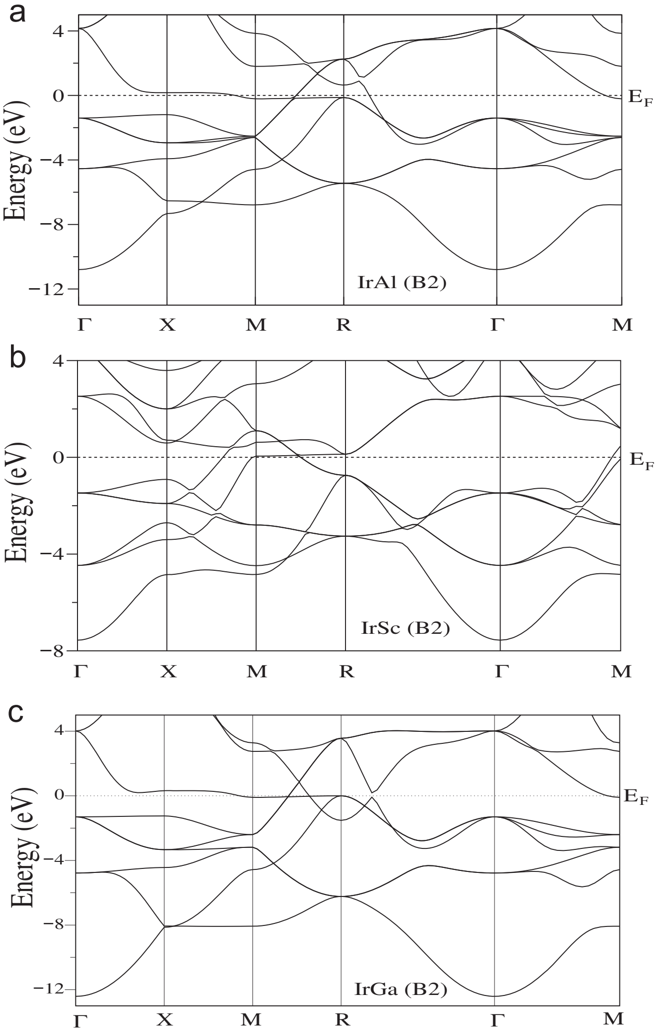

Fig. 1. The electronic band structure for IrX (X=Al, Sc and Ga) compounds along several lines of high symmetry in the Brillouin zone.

ScIr. The density of states at Fermi energy N(E_F) that shows the degree of metallicity of these materials IrX (X=Al, Sc, and Ga) is calculated and it is found to be 0.510, 0.561, and 0.476 states/eV Cell for IrSc, IrAl, and IrGa, respectively. The stability in compounds is associated with the low density of states (DOS) at the Fermi energy E_F hence; we conclude that IrGa is the most stable compound among the studied ones. From our finding values of cohesive energies of IrX (X=Al, Sc, and Ga) compounds which are represented in Table 1, we confirm that IrGa is the most stable compound. The lowest valence bands in the energy region that is lower than −8 eV are mainly due to the "p" electrons of Al (Ga), and the Ir atom for IrAl and IrGa and a mixture of s, p, and d orbitals for IrSc. The states d of the Ir and Sc atoms extend from about −5 to +4 eV and hybridize with each other.

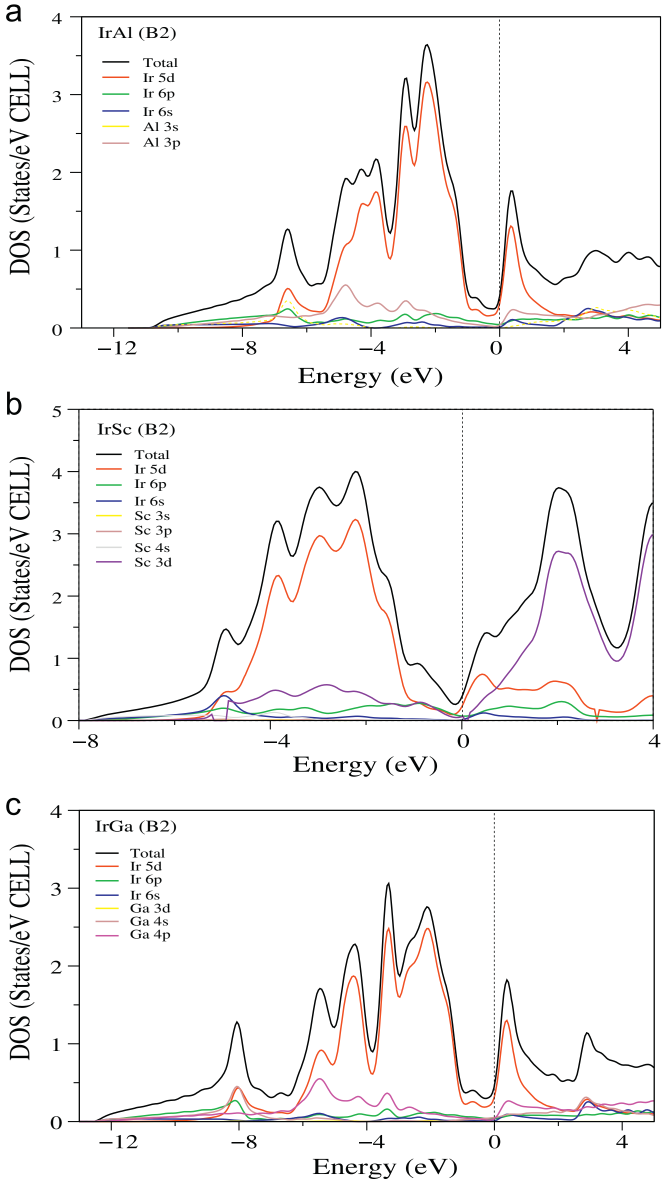

Fig. 2. Calculated partial and total DOS for IrX (X=Al, Sc and Ga) in the B2 phase.

In an attempt to further improve the understanding of the IrX (X=Al, Sc and Ga) compounds, in the present work, we have studied the dynamical properties of IrX (X=Al, Sc, and Ga) alloys, which are calculated by using the density-functional perturbation theory (DFPT). The dynamical matrices can be obtained at arbitrary points in the BZ with the help of a Fourier deconvolution procedure. The CsCl phase iridium alloys belong to the cubic system, with the space group Pm3m. The phonon dispersion curves, total and partial density of states for B2-IrX (X=Al, Sc and Ga) can be seen in Fig. 3. For three alloys, the cesium chloride structure is dynamically stables as throughout the BZ all phonon frequencies are not imaginary. According to the phonon density of states for three alloys, the sharp peaks, which are centered about 3 THz, are due to longitudinal acoustic (LA) and transverse acoustic (TA) phonon modes. The computed phonon density of states for IrSc and IrAl show a band gap between the acoustic and optic branches of around 1.628 and 1.414 THz, respectively. For IrGa, there is no gap between the acoustic and optical branches in the density of states. The contributions to frequency ranges result from significant differences in the atomic weight. The acoustic branches of IrX (X=Al, Sc, and Ga) compounds almost entirely come from Ir

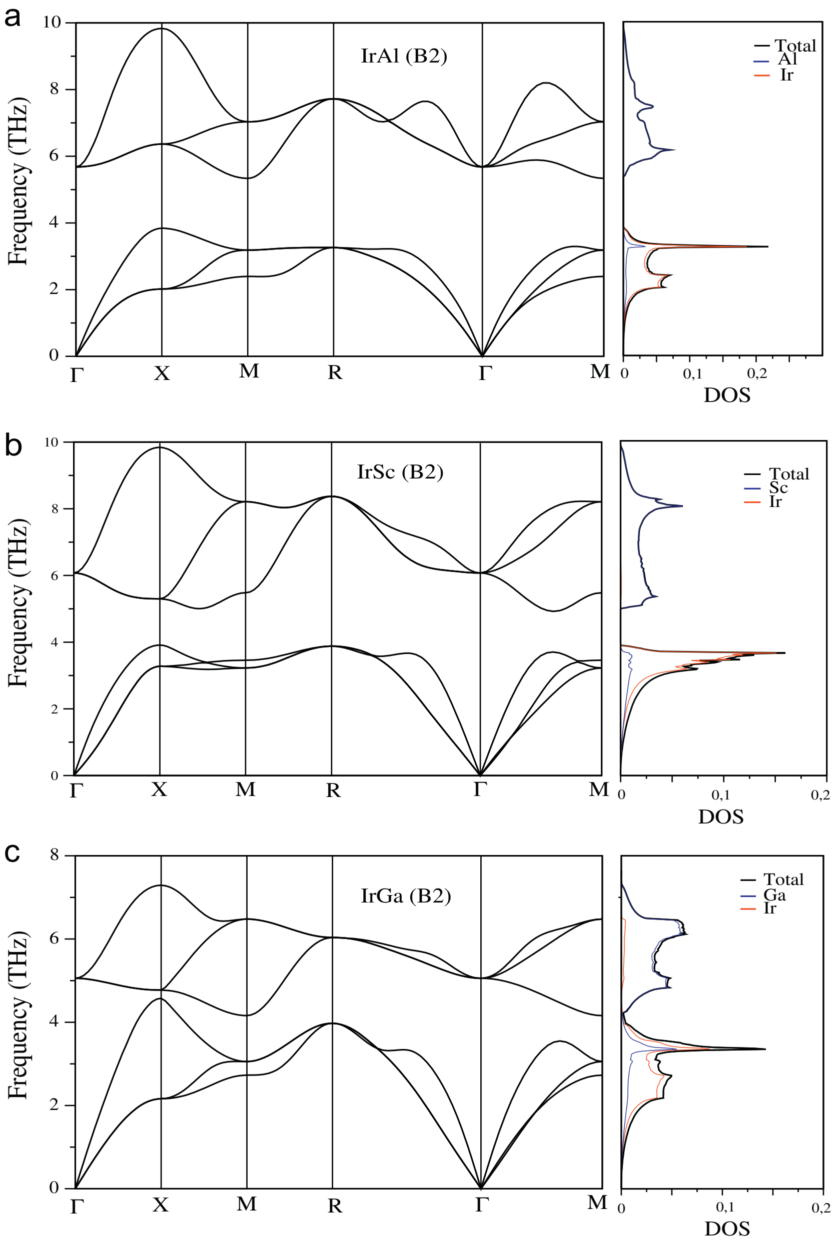

Fig. 3. Phonon dispersion curves and phonon density of states for IrX (X=Al, Sc and Ga) compounds along several lines of high symmetry in the Brillouin zone.

states, whereas the optical branch contains mainly Sc (Ga and Al) states. The optical phonon modes at the zone center of IrSc, IrGa, and IrAl were calculated to be 6.172, 4.749, and 5.639 THz, respectively. It should be noted that phonon dispersion curves of IrX (X=Sc, Ga, and Al) compounds have not yet been theoretically and experimentally studied to the knowledge of the authors.

The calculated specific heat capacity at constant volume (*Cv*), internal energy E, free energy F and entropy S of IrX (X=Al, Sc and Ga) compounds as a function of temperature is shown in Fig. 4. The *Cv* increases rapidly in the range 0–300 K before it starts to saturate. The calculated specific heat capacity *Cv* is very close to the Dulong-Petit limit [30] at a high-temperature, which is commonly satisfied with all solids at high temperatures. For all materials, the *Cv* functions flatten out as the temperature increases above 300 K. Unfortunately, no experimental data are available of the specific heat capacity for these materials. In addition it is clearly seen that the enthalpy E and the entropy S increases with temperature however the Free energy decreases. A small effect of the X atom is shown on the thermodynamic properties of IrX (X=Al, Sc and Ga) compounds, while the *Cv* and the entropy S increases when we move from Ga to Al, The internal energy, free energy F decreases. The same behavior is found in AlY_2 binary compound [43].

4. Conclusion

For long use and high temperature, materials are required to have good phase stability and good mechanical properties such as ductility and toughness as well as oxidation resistance. The aim of this study is to investigate the structural, elastic, electronic and phonon properties of IrX (X=Al, Sc and Ga) compounds. The pseudopotential method was used in the framework of the density functional theory (DFT) with the generalized gradient approximation (GGA). Our calculations show that the lattice constant increases as we progress from IrAl to IrGa to IrSc. On the other

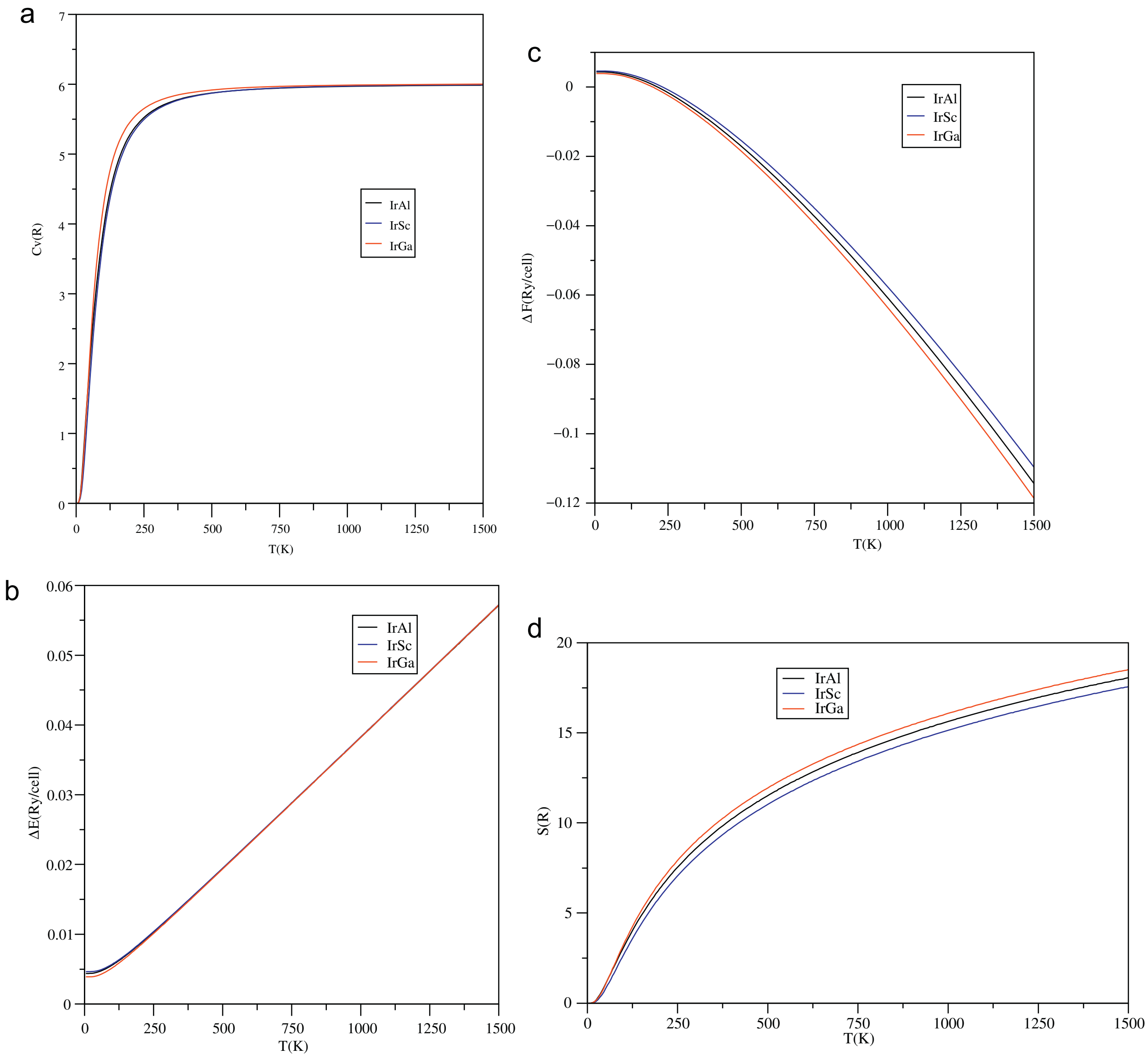

Fig. 4. The specific heats at constant volume (a), internal energy *E* (b), phonon free energy *F* (c) and entropy *S* (d) versus temperature for IrX (X=Al, Sc and Ga) compounds.

hand, the bulk modulus decreases as we move from IrAl to IrGa to IrSc. The bulk modulus decreases by 5% when we replace Al by Ga, and by 26% when we substitute Sc for Al. To quantify the elastic behavior of the materials in question, the elastic constants are calculated from the phonon dispersion curves. Additional mechanical behavior is described by other elastic moduli, such as the shear modulus G, the bulk modulus B, and many others. Our calculated elastic constants are used to check the mechanical stability of the compounds under study. The brittleness and ductility properties of IrX (X=Al, Sc, and Ga) are determined by Poisson's ratio σ criterion and the *B*/*G* ratio. The IrGa compound is a ductile material, whereas IrAl and IrSc show brittleness. The band structure and the electronic densities of states (DOS) of all the compounds are computed, and analyzes are performed. In particular, attention is focused on the behavior of the DOS at the Fermi energy in connection with the stability predicted by the total energy calculations. The contributions of d orbitals to the bands near the Fermi level are discussed. The phonon dispersion curves confirm the mechanical stability of IrX (X=Al, Sc and Ga) compounds. The acoustic branches of IrX (X=Al, Sc, and Ga) alloys almost entirely come from Ir states, whereas the optical branch contains mainly Sc (Ga and Al) states. It is found that the heat capacity, internal energy and entropy increase with temperature,but free energy exhibits different trend.

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