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Research Article

The Effect of Indium Concentration on the Structure and Properties of Zirconium Based Intermetallics: First-Principles Calculations

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The phase stability, mechanical, electronic, and thermodynamic properties of In-Zr compounds have been explored using the first-principles calculation based on density functional theory (DFT). The calculated formation enthalpies show that these compounds are all thermodynamically stable. Information on electronic structure indicates that they possess metallic characteristics and there is a common hybridization between In-p and Zr-d states near the Fermi level. Elastic properties have been taken into consideration. The calculated results on the ratio of the bulk to shear modulus (B/G) validate that $InZr_3$ has the strongest deformation resistance. The increase of indium content results in the breakout of a linear decrease of the bulk modulus and Young's modulus. The calculated theoretical hardness of α-In_3Zr is higher than the other In-Zr compounds.

1. Introduction

Saitovitch et al. made a study on the nuclear probe Cd on In sites of intermetallic compounds of the In-Zr system [1]. However, there is still short of experimental information available on the zirconium-indium system. Experiments on the phase diagram of In-Zr system present the phase compositions of In-Zr compounds [2]. Zumdick et al. examined the crystal structures and properties of $ZrIn_2$ and discussed the chemical bonding of $ZrIn_2$ on the basis of density functional calculations [3]. Meschel and Kleppa studied the standard enthalpies of formation of some transition metal-indium compounds by high-temperature direct synthesis calorimetry and provided some new thermochemical data for In-Zr binary systems [4].

To the best of our knowledge, there is no systematically relevant research on the structural stability and mechanical properties of the In-Zr compounds. Indium possesses unique physical and chemical properties and has been widely applied in the fields of medicine and health, solar battery, national defense and military, aerospace, and modern information industry. The applications of indium compounds and alloys are restricted due to technical level and high cost. Actually, fundamental investigation on indium-related materials is still a challenge.

Recently, advances in computer-aided design and computer-aided manufacturing (CAD/CAM) technology are used in novel manufacturing routes [5]. First-principles calculation is a reliable and precise approach for studying ground-state properties such as the structure, elastic properties, and phase stability. In this paper, we made a systemic investigation on the structure and properties of zirconium based intermetallics. Structural, mechanical, electronic, and thermodynamic properties of four In-Zr compounds have been analyzed and discussed in detail by performing the first-principles calculations. It may improve the knowledge of the In-Zr alloys and provide available theoretical basis for further optimization and design for both indium and zirconium alloys.

2. Computational Methods

All calculations were performed by first principle based on density functional theory (DFT) implemented in Cambridge sequential total energy package (CASTEP) code [6]. The

interaction between ions and electrons was described by using the ultrasoft pseudopotential [7]. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) [8] was used for the exchange correlation functional. The electronic configurations in this study were In $4d^{10}\ 5s^2\ 5p^1$ and Zr $4s^2\ 4p^6\ 4d^2\ 5s^2$, respectively. We choose various k points here mainly because the different phases possess diverse structure. All parameters including k point convergence test have been carefully tested. To ensure the precision of the calculations, we select firstly the k point and cutoff energy at the fine precision as the initial value and then improve continually precision by change the k point and cutoff energy until the calculated crystal parameters have a great agreement with previous data. The corresponding results were displayed in Table 1. According to the calculation at the different k points and cutoff energy, the cutoff energy and k point were selected for different phase. In this work, the cutoff energy of 450 eV was set to InZr and α-In_3Zr and 350 eV was set to In_2Zr. Meanwhile, the cutoff energy of 550 eV was selected for all other phases. Brillouin zone integrations were performed by using a Monkhorst-Pack k point mesh and grids of $12 \times 12 \times 12$, $7 \times 7 \times 7$, $6 \times 6 \times 1$, $6 \times 6 \times 2$, $15 \times 15 \times 10$, and $15 \times 15 \times 8$ k point were set to be the sampling of $InZr_3$, InZr, In_2Zr, α-In_3Zr, In, and α-Zr, respectively. During the structural optimization, all atoms were fully relaxed using conjugate gradient method until the total energy, force, and atomic displacement were less than 1×10^{-5} eV/Å, 0.03 eV/Å, and 0.001 Å, respectively.

Table 1: The lattice constants (Å) of In-Zr compounds at different k points and cutoff energy.

Phase	k points	Energy cutoff (eV)	a (Å)	b (Å)	c (Å)
$InZr_3$	$6 \times 6 \times 6$	350	4.480		
	$6 \times 6 \times 6$	380	4.479		
	$6 \times 6 \times 6$	400	4.479		
	$8 \times 8 \times 8$	400	4.479		
	$8 \times 8 \times 8$	420	4.479		
	$8 \times 8 \times 8$	450	4.479		
	$12 \times 12 \times 12$	450	4.480		
	$12 \times 12 \times 12$	500	4.475		
	$12 \times 12 \times 12$	550	4.474		
InZr	$6 \times 6 \times 6$	350	4.473		
	$6 \times 6 \times 6$	380	4.472		
	$6 \times 6 \times 6$	400	4.471		
	$7 \times 7 \times 7$	400	4.469		
	$7 \times 7 \times 7$	420	4.470		
	$7 \times 7 \times 7$	450	4.470		
	$8 \times 8 \times 8$	400	4.471		
	$8 \times 8 \times 8$	420	4.471		
	$8 \times 8 \times 8$	450	4.471		
In_2Zr	$6 \times 6 \times 1$	350	4.442		27.890
α-In_3Zr	$6 \times 6 \times 1$	350	4.371		19.514
	$6 \times 6 \times 1$	400	4.358		19.349
	$6 \times 6 \times 1$	450	4.364		19.318
	$6 \times 6 \times 2$	350	4.370		19.514
	$6 \times 6 \times 2$	400	4.359		19.339
	$6 \times 6 \times 2$	450	4.364		19.293

3. Results and Discussions

3.1. Structural Stability. In this section, we established the initial crystal structures of four In-Zr compounds based on the experimental crystallographic data. Then the lattice parameters and internal coordinates of these compounds were optimized with the measure of first-principle calculation. Figure 2 presents the optimized structural models of four In-Zr compounds and Table 2 lists the lattice parameter compared with the available experimental data. The reliability of this work and the reasonability of the computational methodology can be justified from the good agreement between the available experimental data and present work in optimized lattice parameters and atomic coordinates.

The enthalpy of formation was calculated in this part so as to estimate the thermodynamic stability of In-Zr compounds. Enthalpy of formation of In-Zr compounds is defined as follows:

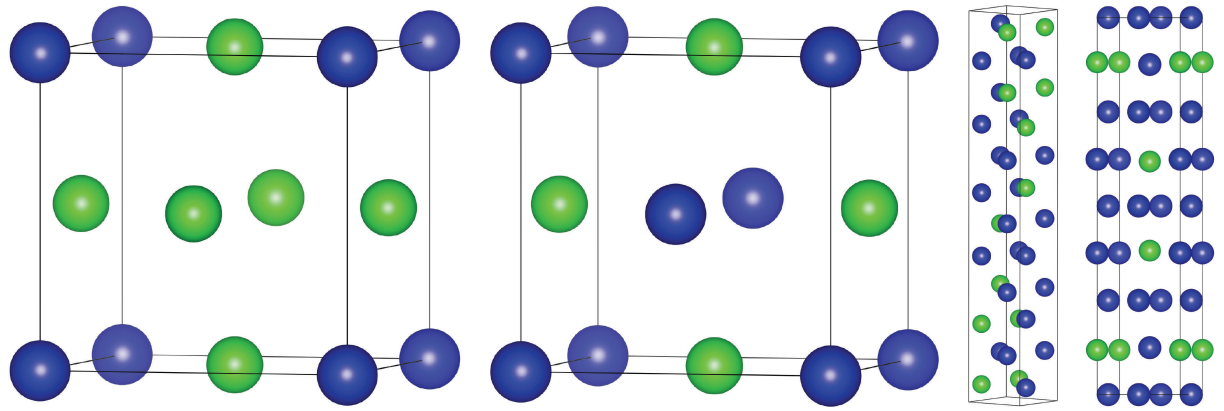
$$\Delta H = \frac{E_{\text{total}} - xE_{\text{In}}^{\text{bulk}} - yE_{\text{Zr}}^{\text{bulk}}}{x + y}, \tag{1}$$

where E_{total} is the total energy of In_xZr_y and $E_{\text{In}}^{\text{bulk}}$ and $E_{\text{Zr}}^{\text{bulk}}$ are the total energy of an indium atom and a zirconium atom in the bulk state, respectively. The calculated results are listed in Table 2. The obtained formation enthalpies of the In-Zr compounds are all negative, meaning that they are all stable at 0 K and 0 GPa [13]. We can see that the formation enthalpy of InZr is the lowest contrast with α-In_3Zr, In_2Zr, and $InZr_3$, which implies that InZr is the most stable among four Zr-In compounds.

3.2. Mechanical Properties. Before considering the mechanical properties, we prefer to study the mechanical stability of these In-Zr compounds. According to the structural feature (see Figure 1), the compounds discussed in this paper mainly consist of two crystal structures such as cubic structure (i.e., $InZr_3$ and InZr) and tetragonal structure (i.e., In_2Zr and α-In_3Zr). For the cubic crystal, there are three independent elastic constants, that is, C_{11}, C_{12}, and C_{44}. Counterpart criterion of mechanical stability is based on the following formula [14]:

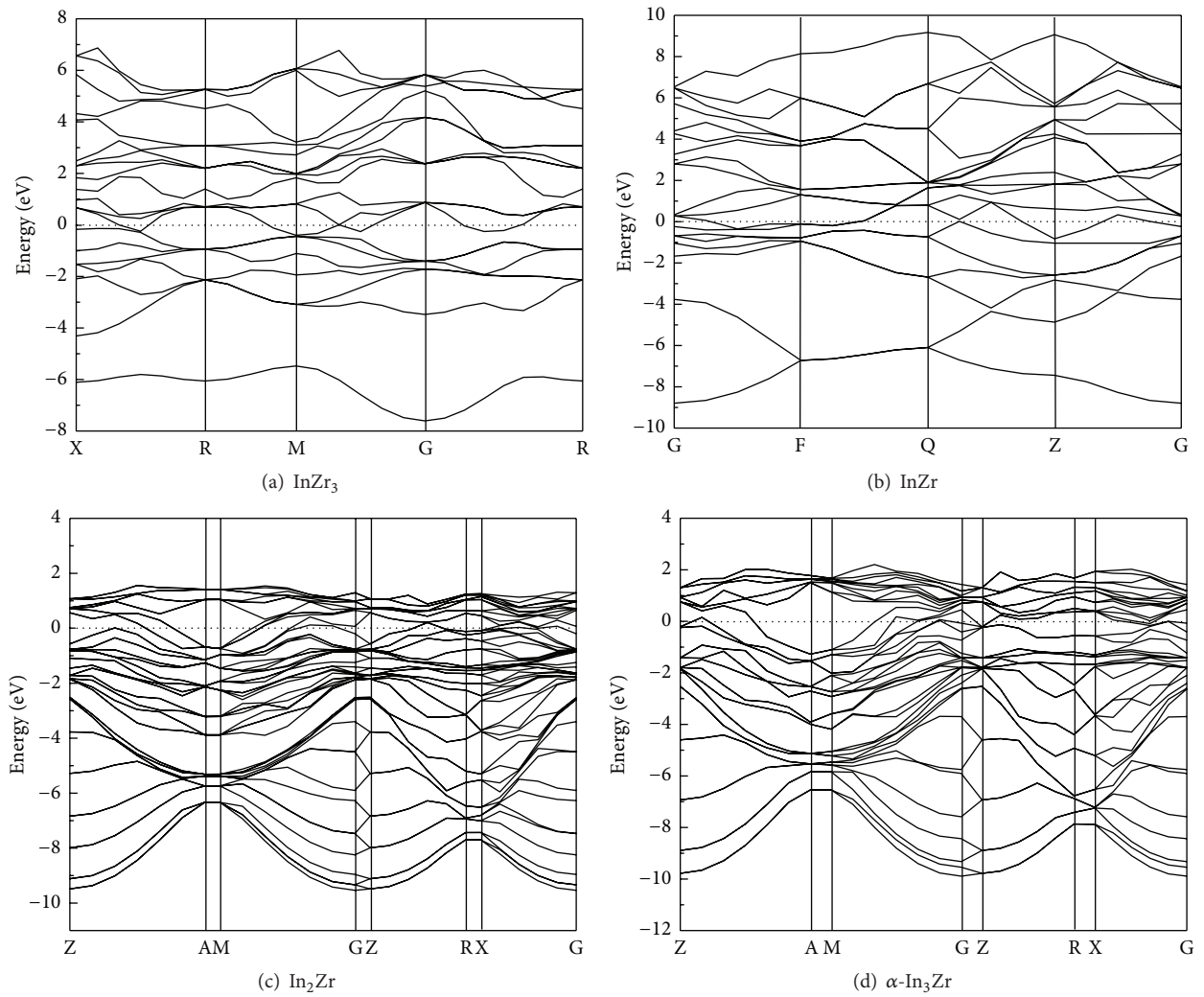
$$\begin{aligned} C_{11} &> 0; \\ C_{44} &> 0; \\ C_{11} &> \left|C_{12}\right|; \\ \left(C_{11} + 2C_{12}\right) &> 0. \end{aligned} \tag{2}$$

For tetragonal system, there are six independent elastic constants, that is, C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, and C_{66}. The



(a) $InZr_3$ (b) InZr (c) In_2Zr (d) α-In_3Zr

FIGURE 1: Structure model of In-Zr compounds. (a) $InZr_3$, (b) InZr, (c) In_2Zr, and (d) α-In_3Zr. Blue and green spheres represent In and Zr atoms, respectively.



(a) $InZr_3$ (b) InZr (c) In_2Zr (d) α-In_3Zr

FIGURE 2: The electronic energy band structures near Fermi level of In-Zr intermetallics. The dotted lines denote the Fermi level E_F.

Table 2: Calculated lattice parameters (Å) and formation enthalpies (eV/atom) for In, α-Zr, and In-Zr intermetallic compounds in comparison with the available experimental data.

Phase	Space (number)	Prototype	Pearson's symbol	Atomic numbers	a	b	c	Formation enthalpy (eV/atom)
$InZr_3$	Pm-3m (221)	$AuCu_3$	cP4	4	4.474 4.450 [2] 4.461 [9] 4.460 [10]			−0.247
InZr	Fm-3m (225)	Cu	cF4	4	4.47 4.418 [2]			−0.313
In_2Zr	I41/amdZ (141)	$HfGa_2$	tI24	24	4.442 4.385 [2] 4.387 [3]		27.89 27.23 27.238	−0.284
α-In_3Zr	I4/mmm (139)	Al_3Zr	tI16	16	4.364 4.303 [2]		19.293 18.94	−0.212
In	I4/mmm (139)	In	tI2	2	3.271 3.251 [2] 3.251 [11]		5.172 4.947 4.947	
α-Zr	P63/mmc (194)	Mg	hP2	2	3.23 3.232 [12] 3.232 [2]		5.175 5.148 5.148	

qualification for stability can be measured in the following expression [14]:

$$\begin{aligned} C_{11} &> 0;\\ C_{33} &> 0;\\ C_{44} &> 0;\\ C_{66} &> 0;\\ C_{11} - C_{12} &> 0;\\ C_{11} + C_{33} - 2C_{13} &> 0;\\ 2\left(C_{11} + C_{12}\right) + C_{33} + 4C_{13} &> 0. \end{aligned} \tag{3}$$

Elastic constants reflect the resistance of a crystal to an applied external stress, whose values will provide valuable information about structural stability [15]. Based on the calculation results, all the In-Zr compounds conform to the corresponding standard of stability. That is, the In-Zr compounds considered in this paper are all mechanically stable. The mechanical prospects for all compounds show that four Zr-In intermetallic compounds have stable structure [16].

For researching the mechanical properties of the In-Zr compounds, the following computational formulas are used [17]:

$$\begin{aligned} B &= \frac{1}{2}\left(B_V + B_R\right),\\ G &= \frac{1}{2}\left(G_V + G_R\right),\\ E &= \frac{9GB}{3B + G}. \end{aligned} \tag{4}$$

For cubic system [17],

$$\begin{aligned} B_V &= B_R = \frac{1}{3}\left(C_{11} + 2C_{12}\right),\\ G_V &= \frac{1}{5}\left(C_{11} - C_{12} + 3C_{44}\right),\\ G_R &= \frac{5\left(C_{11} - C_{12}\right)C_{44}}{3\left(C_{11} - C_{12}\right) + 4C_{44}}. \end{aligned} \tag{5}$$

Particularly, the InZr compound breaks the symmetry of the cubic system, and the general elastic constants are [18]

$$\begin{aligned} \overline{C_{11}} &= \frac{C_{11} + C_{22} + C_{33}}{3},\\ \overline{C_{12}} &= \frac{C_{12} + C_{13} + C_{23}}{3},\\ \overline{C_{44}} &= \frac{C_{44} + C_{55} + C_{66}}{3}. \end{aligned} \tag{6}$$

For tetragonal system [14],

$$\begin{aligned} B_V &= \frac{2\left(C_{11} + C_{22}\right) + C_{33} + 4C_{13}}{9},\\ G_V &= \frac{M + 3C_{11} - 3C_{12} + 12C_{44} + 6C_{66}}{30},\\ B_R &= \frac{C^2}{M},\\ G_R &= \frac{15}{\left[18B_V/C^2 + 6/\left(C_{11} - C_{12}\right) + 6/C_{44} + 3/C_{66}\right]},\\ M &= C_{11} + C_{12} + 2C_{33} - 4C_{13},\\ C^2 &= \left(C_{11} + C_{12}\right)C_{33} - 2C_{13}^2. \end{aligned} \tag{7}$$

From Table 4, it can be seen that $InZr_3$, with the bulk modulus of 97.112 GPa, has the strongest resistance to volume change by applied pressure [19] and the strongest average bond strength of atoms for the given crystal [20]. On the contrary, α-In_3Zr is the weakest one compared with the other In-Zr compounds. As shown in Table 4 the relation between bulk modulus and indium content is monotonically decreasing, which is equivalent to the resistance to volume deformation of the four compounds and the abrupt degradation of average bond strength of atoms with increasing indium content. The shape change capacity of material is usually reflected in the value of shear modulus [15]. The difference of this value between $InZr_3$ and α-In_3Zr is quite small. The lowest shear modulus is 47.007 GPa for InZr and the highest shear modulus is only 51.6 GPa for $InZr_3$. There is no obvious rule about shear modulus with increasing indium content. What is more, it can be seen that $B > G$ exists in the In-Zr system, indicating that shear modulus limits the mechanical stability of the In-Zr compounds [21]. Materials with high Young's modulus depict strong resistance to uniaxial tension [22] and indicate the elastic stiffness as well. It can be seen from Table 4 that calculated Young' modulus of $InZr_3$ is 131.509 GPa, which is higher than that of the other In-Zr compounds. Young's modulus of α-In_3Zr is only about 118.350 GPa, which is lower than all the others. We can conclude from above analysis that E has similar change compared with B. Young's modulus decreases linearly with increasing indium content. In addition, it should be noted that C_{12} and C_{44} are much lower than C_{11} for all compounds, which implies that all the crystals are more difficult to deform in the axial direction, compared with shear direction [23].

B/G ratio, in general, was applied to describe the brittleness and toughness of materials [24]. The brittle-ductile transition of materials can be judged by the B/G ratio. If the B/G ratio exceeds 1.75, the material is ductile. Otherwise, it is brittle. From Table 4, the B/G value of α-In_3Zr is less than 1.75, which implies the brittleness of this compound. The B/G values of $InZr_3$, InZr, and In_2Zr are all higher than 1.75, demonstrating that these In-Zr intermetallic compounds are ductile. Poisson's ratio ν can be used to forecast the ductility of crystals, as well [25]. From Table 4, it is shown that B/G and ν have similar variation trend with increasing Zr content. It is found that when B/G is higher than 1.75, the values of ν are more than 0.26 for $InZr_3$, InZr, and In_2Zr. This is consistent with the conclusion that ductile compounds usually have high ν.

The hardness parameter H can be calculated [26]:

$$H = \frac{(1-2\nu)E}{6(1+\nu)}, \qquad \nu = \frac{3B-2G}{2(3B+G)}. \tag{8}$$

The calculated theoretical hardness was shown in Table 4. We can know that there is a transition at 0.67 indium content. When indium content is less than 0.67, the hardness may decrease with increasing indium content. While it is higher than 0.67, hardness exhibits a big jump and increases with the indium increasing. The calculated theoretical hardness of α-In_3Zr is 15.809, which indicates that α-In_3Zr is expected to be the hardest among all the In-Zr binary compounds.

Table 3: Calculated elastic constants C_{ij} (GPa) for In-Zr compounds.

Phase	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
$InZr_3$	140.589	75.373			70.192	
InZr	129.626	74.343			67.083	
In_2Zr	124.925	63.411	49.866	224.796	42.994	56.707
α-In_3Zr	129.757	53.044	42.007	172.837	40.61	63.057

Table 4: The calculated shear modulus G (GPa), bulk modulus B (GPa), Young's modulus E (GPa), bulk modulus to shear modulus ratio (B/G), Poisson's ratio, and Hardness (GPa) as well as available experimental and theoretical data.

Phase	B	G	E	H	ν	B/G
$InZr_3$	97.112	51.6	131.509	7.764	0.274	1.882
InZr	92.771	47.007	120.644	6.792	0.283	1.974
In_2Zr	87.104	47.184	119.903	15.728	0.271	1.846
α-In_3Zr	78.18	47.427	118.35	15.809	0.248	1.648

3.3. Electronic Properties. In order to study the electronic properties of the In-Zr intermetallic compounds, we calculate the electronic energy band structures and the results are depicted in Figure 2, where the dot dash line zero-point energy signifies the highest energy level occupied by the valence electrons at 0 K. From Figure 2, we can know that all compounds show metallic nature due to the fact that these bands cross E_F. Meanwhile, the density of states corresponding to the Fermi surface was all positive, which also implies that all these In-Zr intermetallics are conductive phases.

To further understand the electronic structure and mechanical properties of four In-Zr compounds, density of states was calculated and analyzed in detail. Figure 3 represents the total and partial density of states of four In-Zr compounds, where the black vertical dashed of DOS indicates the Fermi level (E_F). As is vividly demonstrated in Figure 3, the valence electron near E_F mainly derived from In-p and Zr-d states. It indicates that the 5p states of In hybridize strongly with the Zr 4d states and the In-Zr atomic bonds formed along the p-d directions near the region Fermi level. Particularly, the DOS profile of $InZr_3$ presents an obvious pseudogap. The pseudogap indicates that the hybridization between In and Zr induces a separation of the bonding states and antibonding states [13]. That is why $InZr_3$ own the greatest deformation resistance [27].

The distance between the zero energy symbolized bands and the nearest peaks may manifest the bonds transformation of compounds [28, 29]. In general, the longer the distance to the zero energy symbolized bands, the stronger the covalent bonds. Moreover, with the falling in metallicity of bond, alloy ductility usually decreases [30]. As the DOS shown in Figure 3, the distance adjacent zero energy is the lowest

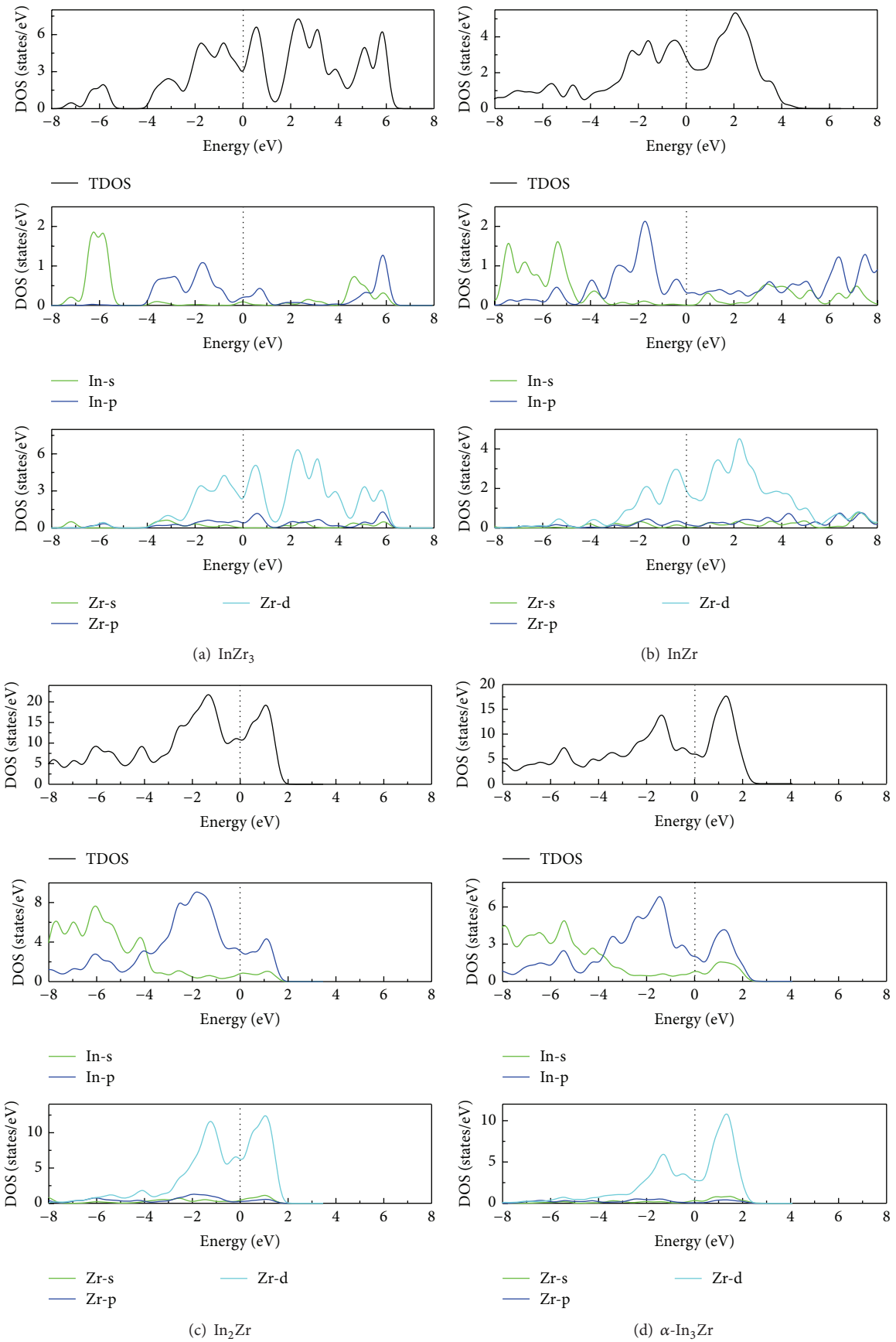


Figure 3: Total and partial electronic densities of states near Fermi level of In-Zr intermetallics. The dotted lines denote the Fermi level E_F.

for InZr among these binary In-Zr phases, implying that it possesses the strongest metallicity and hence it has the best ductility. This result has a well consistency with the ductility estimated from the G/K and Poisson's ratio values.

Furthermore, we can estimate the structural stability of intermetallic compounds through different density of states at the Fermi levels [16]. Usually, the lower the value at Fermi levels, the more strong the stability of the structure. From Figure 3, InZr has the minimum value of density of states and in consequence has the most stable structure, which has a great consistency to our results of formation enthalpy.

3.4. Thermodynamic Properties. Debye temperature was calculated to provide insight into the thermodynamics behaviors. The values of Young's modulus, bulk modulus, and shear modulus were obtained from the above section and then put into the following formula [16]:

$$\begin{aligned}
\Theta_D &= \frac{h}{k}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3} v_m,\\
v_m &= \left[\frac{1}{3}\left(\frac{2}{v_s^3}+\frac{1}{v_l^3}\right)\right]^{-1/3},\\
v_l &= \sqrt{\frac{B+(4/3)\,G}{\rho}},\\
v_s &= \sqrt{\frac{G}{\rho}},
\end{aligned} \tag{9}$$

where Θ_D is Debye temperature, h is Planck's constant, k is Boltzmann's constant, n is the number of atoms per formula, M is the molecular weight, v_m, v_l, and v_s are the average wave velocity, the longitudinal, and shear velocity, respectively, and ρ is the theoretical density of the compound. B and G are the bulk modulus and shear modulus, respectively. The values of Debye temperature, average wave velocity, longitudinal, and shear wave velocity for each compound are listed in Table 5. As we all know the strength of chemical bonding can be characterized by Debye temperature which is inverse to the molecular weight [16, 23]. Stronger chemical bonding favors higher Debye temperature. As shown in Table 5, we can find that the highest Θ_D value is 314.9 K for $InZr_3$, and the lowest one is ascribed to α-In_3Zr. Therefore, we can conclude that the covalent bonds in $InZr_3$ are stronger than the others.

4. Conclusions

In summary, we have performed first-principle calculations to investigate the structural, mechanical, electronic, and thermodynamic properties of In-Zr compounds with different indium concentrations. The calculated results show that the lattice parameters of all compounds are in good agreement with the obtained experimental data and theoretical results. The calculated formation enthalpy indicates that InZr is more stable than the others.

Table 5: Sound velocity, density, and Debye temperature of In-Zr compounds.

Phase	Density (g/cm^3)	v_s	v_l	v_m	Θ_D
$InZr_3$	7.201	2676.875	4800.011	2980.477	314.897
InZr	7.662	2476.89	4504.19	2760.842	291.892
In_2Zr	7.747	2467.895	4400.46	2746.552	287.773
α-In_3Zr	7.876	2453.963	4237.448	2723.632	285.176

The calculated elastic constants show that all the compounds are mechanically stable (Table 3). The bulk modulus and Young's modulus decrease linearly with increasing indium content. The calculated shear modulus and Young's modulus of $InZr_3$ are 51.6 GPa and 131.509 GPa, respectively, which are higher than the other compounds. All In-Zr compounds exhibit ductile behavior but α-In_3Zr exhibits brittle behavior. We conclude that the variation of mechanical properties is related not only to the indium concentration, but also to the bonding state in the In-Zr compounds.

Competing Interests

The authors declare that they have no competing interests.

Acknowledgments

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