

Article

First-Principles Investigations on Structural Stability, Elastic Properties and Electronic Structure of $\text{Mg}_{32}(\text{Al},\text{Zn})_{49}$ Phase and MgZn_2 Phase

Yu Song^{1,2}, Songtao Zhan^{1,2}, Baohua Nie^{1,2,*} , Haiying Qi^{1,2}, Fangjun Liu³, Touwen Fan⁴ and Dongchu Chen^{1,2,*}

- ¹ School of Materials Science and Hydrogen Energy, Foshan University, Foshan 528000, China; songyu188200@foxmail.com (Y.S.); 20200580229@stu.fosu.edu.cn (S.Z.); haiyingqi@fosu.edu.cn (H.Q.)
² Guangdong Key Laboratory for Hydrogen Energy Technologies, Foshan 528000, China
³ School of Mechatronic Engineering and Automation, Foshan University, Foshan 528000, China; lfj816@126.com
⁴ College of Science, Hunan Institute of Technology, Hengyang 421002, China; fantouwen@hotmail.com
* Correspondence: niebaohua121@163.com (B.N.); cdcever@163.com (D.C.); Tel.: +86-0757-82700525 (B.N.); +86-0757-82700525 (D.C.)

Abstract: Al–Mg–Zn alloys reinforced by T– $\text{Mg}_{32}(\text{Al},\text{Zn})_{49}$ phase had higher structure stability and strength than Al–Zn–Mg–(Cu) alloys reinforced by MgZn_2 phase, but the reasons for these two kind of alloys was not well-known. To reveal the discrepancy between T phase and MgZn_2 phase, the lattice parameters, cohesive energy, and electronic structure as well as the elastic properties were investigated based on density functional theory. Four types of T phase unit cell were employed according to symmetry of space group. The calculated lattice constants well-agreed with experimental data. Compared to MgZn_2 phase, T phases obtained lower cohesive energy owing to their partial covalent bond, which may result in a higher structure stability. The elastic modulus E of T phase depended on the occupation of Al atom, and the effect of the occupation of Al atom on the structure and properties of T phase was also discussed.

Keywords: $\text{Mg}_{32}(\text{Al},\text{Zn})_{49}$; MgZn_2 ; structural stability; elastic properties; electronic structure



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1. Introduction

Al–Zn–Mg–(Cu) aluminum alloys strengthened by MgZn_2 phase are widely used in aerospace and automotive contexts due to their high specific strength. However, typical Al–Zn–Mg–(Cu) aluminum alloys, such as 7075, 7050, and 7055 alloys, have poor corrosion resistance [1], as there is an electrode potential difference between MgZn_2 phase and aluminum matrix. Furthermore, MgZn_2 phase tended to coarsen at high temperature, resulting in a low thermal stability [2], limiting their application in high-temperature parts.

Recently, investigation of Al–Mg–Zn alloys reinforced by T– $\text{Mg}_{32}(\text{Al},\text{Zn})_{49}$ phase has attracted the attention of researchers at home and abroad [3–5]. The research by Zhang [6,7] showed that Al–Mg–Zn alloy obtained a higher strength and toughness than the commercial 7000 series aluminum alloy owing to the strength of T phase. Takata [8] proposed that $\text{Al}_5\text{Mg}_{3.5}\text{Zn}(\text{at}\%)$ alloy has a higher heat resistance than 7055 alloy. Although the microstructure properties of aluminum alloys strengthened by T phase and MgZn_2 phase have been reported [9–11], there are few reports on the discrepancy between T phase and MgZn_2 phase to reveal the reasons for the high strength and structure stability of Al–Mg–Zn alloys.

The electronic structure of MgZn_2 phase was studied based on first-principles calculations. The electronic structure of MgZn_2 phase was analyzed in terms of band structure, density of states and electron density [12]. A systematic investigation of coherent interfaces of MgZn_2 phase was studied using the first-principles method [13]. The electronic

structure and pseudogap of T phase were also investigated on the basis of the quasicrystal model; however, the mechanical properties and electronic structure of T phase were not well known.

In this paper, 1/1 approximant structural [14] of $\text{Mg}_{32}(\text{Al,Zn})_{49}$ phase was employed, which was cubic with space group $\text{Im}\bar{3}$ containing 162 atomic sites. The electronic structures of $\text{Mg}_{32}(\text{Al,Zn})_{49}$ phase and MgZn_2 phase were compared by ab initio methods, and the differences elastic properties of $\text{Mg}_{32}(\text{Al,Zn})_{49}$ phase and MgZn_2 phase were revealed at the atomic scale, providing the theoretical basis for the development of new high-performance aluminum alloys.

2. Computational Method

The first-principles calculation was carried out based on density functional theory (DFT) [15] using the software VASP [16]. The interaction between electrons and ions was described using the projection-augmented wave (PAW) method [17]. The electron configuration was described by $3\text{S}^23\text{P}^1$, 3S^2 and $3\text{d}^{10}4\text{s}^2$ valence states for Al, Mg and Zn, respectively. The Perdew–Burke–Ernzer (PBE) [18] method of generalized gradient approximation (GGA) [19] was used to describe the exchange–correlation energy functional between electrons. The cut-off energy of the plane wave function of electrons was set at 400 eV, and Monkhorst–Pack k-point grids for the Brillouin-zone integration were applied with linear Kmesh-resolved value of less than $0.03\ 2\pi\text{\AA}^{-1}$ along each periodic direction in reciprocal space, to optimize the geometry and calculate elastic constants. Furthermore, the density of states (DOS) was calculated on the condition of less than $0.015\ 2\pi\text{\AA}^{-1}$ along each periodic direction in reciprocal space.

Crystal structures of MgZn_2 and T phases were shown in Figure 1. MgZn_2 phase belonged to the hexagonal structure with the space group $\text{P6}_3/\text{mmc}$, and T-phase model in this calculation had eight sites (A–H) [20], among which Al atoms occupied one position in A and Mg occupied D, E, G, and H positions without any chemical disorder. The Al and Zn atoms usually occupied the B, C, and F atomic sites with chemical disorder. This atomic structure involved a large amount of chemical disorder on sites B, C, and F. Such chemical disorder was eliminated to carry out efficient calculations.

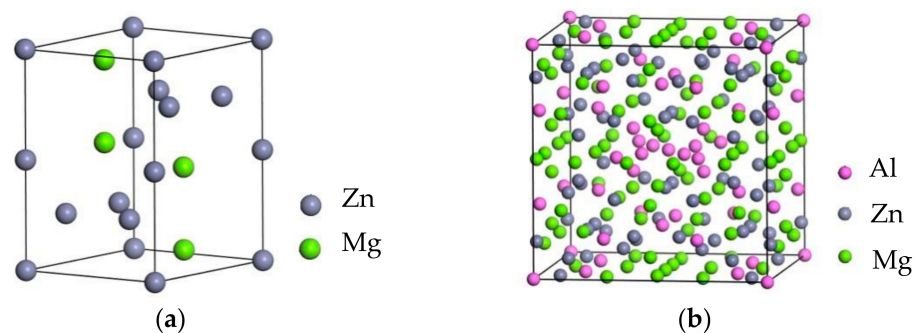


Figure 1. Crystal structure: (a) MgZn_2 ; (b) $\text{T}-(\text{Al,Zn})_{98}\text{Mg}_{64}$.

According to the symmetry of $\text{Im}\bar{3}$ space group (cubic crystal), four configurations of Al: Zn: Mg = 13: 36: 32 and Al: Zn: Mg = 25: 24: 32 were constructed, as Al and Zn atoms occupied site B, C, and F sites respectively [14]. The space group of the calculation model and the space occupying situation were shown in the Table 1.

Table 1. The model structure of T phases.

Sum	Space Group	Sites		
		B (24 g)	C (24 g)	F (48 h)
Al ₂₆ Zn ₇₂ Mg ₆₄ -C	Im3	Zn	Al	Zn
Al ₂₆ Zn ₇₂ Mg ₆₄ -B		Al	Zn	Zn
Al ₅₀ Zn ₄₈ Mg ₆₄ -F		Zn	Zn	Al
Al ₅₀ Zn ₄₈ Mg ₆₄ -BC		Al	Al	Zn

3. Results and Discussion

3.1. Crystal Structure and Stability

In order to ensure the accuracy of the study, the geometric structure of the crystal structure was firstly optimized, and the lattice constants after optimization were listed in Table 2 in comparison with the results of other authors using the same calculation method. It showed that the optimized lattice constants were well-consistent with the experimental values and calculated values.

The cohesive energy (E_{coh}) was a measure of the force to bind atoms together in the solid state, so it showed the structural stability of the alloys. It can be calculated by Formula (1) [21].

$$E_{\text{coh}} = \frac{E_{\text{total}} - n_A E_A^{\text{isolate}} - n_B E_B^{\text{isolate}}}{n_A + n_B} \quad (1)$$

where E_{total} was the total energy of the unit cell and E_A^{isolate} , E_B^{isolate} were the total energies of the isolated A and B atoms in the free state.

The equilibrium formation enthalpy (ΔH) of a compound can refer to the energy consumed for a crystal decomposed into pure crystal elements at equilibrium status. If the equilibrium formation enthalpy of crystal mesophase was lower, the ability of alloying elements composed of this phase was stronger [22].

$$\Delta H = \frac{E_{\text{total}} - n_A E_A^{\text{bluk}} - n_B E_B^{\text{bluk}}}{n_A + n_B} \quad (2)$$

where E_A^{bluk} , E_B^{bluk} were the energy per atom of pure elements at equilibrium status. n_A and n_B referred to the number of A and B atoms in unit cell, respectively.

Considering the precipitation of MgZn₂ phase and T phase from Al solid solution, the fcc-based formation enthalpy (ΔH^{fcc}) of these phases can be calculated as follow [23]:

$$\Delta H^{\text{fcc}} = \frac{E_{\text{total}} - n_A E_A^{\text{fcc}} - n_B E_B^{\text{fcc}}}{n_A + n_B} \quad (3)$$

where E_A^{fcc} , E_B^{fcc} were the per atom energies of A and B in the fcc state. The fcc-based formation enthalpy eliminated the promotion energy, promoting a constituent from its equilibrium structure to the fcc structure [23].

As shown in Table 2, compared with the calculation of the equilibrium formation enthalpies, the fcc-based formation enthalpies of each phase were lower as the elimination of the promotion energy, but still had the similar change trend. T phase obtained higher formation enthalpy than that of MgZn₂ phase, but had lower cohesive energy, indicating that the T phase was more difficult to form, and gained higher melting point and thermal stability. As for T phase, the formation enthalpy gradually increased with increase in Al atoms and decrease in Zn, implying that T phase was difficult to form. However, there was a decreasing tend for the cohesive energy, resulting in higher thermal stability.

Table 2. Lattice parameters, cohesive energy E_{coh} , and formation enthalpy ΔH of the phases T-phase, MgZn_2 .

Phase	Sum	Source	Lattice Parameter/Å			$E_{\text{coh}}/(\text{kJ}\cdot\text{mol}^{-1})$	$\Delta H/(\text{kJ}\cdot\text{mol}^{-1})$	$\Delta H_{\text{fcc}}/(\text{kJ}\cdot\text{mol}^{-1})$
			a	b	c			
MgZn_2	Mg_4Zn_8	This work	5.187	-	8.561	−132.617	−13.186	−14.849
		Ref [24]	5.208	-	8.506	−132.628	−13.346	-
		Exp [25]	5.221	-	8.567	-	-	-
T	$\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-C}$	This work	14.17	-	-	−172.040	−9.728	11.158
	$\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-B}$		14.23	-	-	−169.8	−7.488	−8.918
	$\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-F}$		14.32	-	-	−206.406	−6.952	−8.013
	$\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-BC}$		14.37	-	-	−204.836	−5.319	−6.444
	$\text{Al}_6\text{Zn}_{11}\text{Mg}_{11}$	Exp [8]	14.20	-	-	-	-	-

On the other hand, the occupation of Al and Zn significantly effected the formation enthalpy and the cohesive energy. As for T- $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}$ phase, both the formation enthalpy and the cohesive energy of the occupation site C by Al atom were lower than that of site B, thus Al atom was inclined to occupy site C. Similarly, Al atom in T- $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}$ phase occupied site F with higher probability, and B, C were not simultaneously occupied. The calculated result was consistent with the experimental data, where the atom occupation probability was summarized as B (83.4% Zn, 16.6%Al), C (51%Zn, 49% Al), F (48% Zn, 52%Al) [20].

3.2. Elastic Properties

The elastic constant described the stiffness of the crystal in response to the applied strain [26]. When the strain was very small, the energy of the system had a quadratic linear relationship with the strain (Hooke's law). Based on the energy–strain relationship, a certain elastic constant or a combination of the elastic constants of crystal can be obtained by applying strain in different orientations and sizes to the system, and finally the elastic constant matrix of crystal can be obtained. The specific calculation results of phase elastic constants in this work were shown in Table 3.

Table 3. Calculated elastic constants of phases MgZn_2 and T phase, C_{ij} /GPa.

Phase	Sum	Source	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
MgZn_2	MgZn_2	This work	117.26	52.91	34.67	109.29	28.41	32.17
		Ref [27]	119.48	42.98	30.04	129.48	24.23	38.25
		Exp [28]	107.25	45.45	27.43	126.40	27.70	30.9
T-phase	$\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-C}$	This work	128.91	54.96	-	-	42.54	-
	$\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-B}$		116.61	53.73	-	-	29.94	-
	$\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-F}$		126.02	58.02	-	-	35.92	-
	$\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-BC}$		128.91	54.96	-	-	42.54	-

Based on the calculated quadratic elastic coefficient matrix, the elastic properties of polycrystalline systems can be obtained using Voigt–Reuss–Hill approximation [29]. According to Born–Huang's lattice dynamical theory, the mechanical stability criterion can be expressed as:

Hexagonal system:

$$C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0, (C_{11} + C_{12}) \times C_{33} > 2C_{13}^2 \quad (4)$$

Cubic system:

$$C_{11} > 0, C_{12} > 0, C_{44} > 0, C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0 \quad (5)$$

MgZn₂ phase is a hexagonal P6₃/mmc system with six independent constants (C_{11} , C_{12} , C_{13} , C_{33} , C_{44} and C_{66}), in which $C_{66} = (C_{11} - C_{12})/2$. The Voigt and Reuss boundary values of hexagonal crystal system (MgZn₂) were calculated by the following formula [30].

$$M = C_{11} + C_{12} + 2C_{33} - 4C_{13} \quad (6)$$

$$N = (C_{11} + C_{12}) \times C_{33} - 2C_{13}^2 \quad (7)$$

$$B_v = \frac{2(C_{11} + C_{12}) + 4C_{13} + C_{33}}{9} \quad (8)$$

$$G_v = \frac{M + 12(C_{44} + C_{66})}{30} \quad (9)$$

$$B_r = \frac{N}{M} \quad (10)$$

$$G_r = \frac{5NC_{44}C_{66}}{2 \times [3B_vC_{44}C_{66} + N(C_{44} + C_{66})]} \quad (11)$$

where the B indicates bulk modulus, G is shear modulus, and the subscripts v and r indicate the Voigt and Reuss values, respectively.

T phase is Im3 structure and belongs to the cubic crystal. There are only three independent elastic constants (C_{11} , C_{12} and C_{44}). The bulk modulus and shear modulus of the cubic crystal system can be calculated by the equations [31].

$$B = B_v = B_r = \frac{C_{11} + 2C_{12}}{3} \quad (12)$$

$$G_v = \frac{3C_{44} + C_{11} - C_{12}}{5} \quad (13)$$

$$G_r = \frac{5(C_{11} - C_{12}) \times C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \quad (14)$$

The Voigt–Reuss–Hill approximations, averaging Voigt and Reuss, were considered as the best estimation of the theoretical polycrystalline elastic modulus. The polycrystalline Young's modulus and Poisson's ratio can be calculated from the values of elastic modulus as follows [32]:

$$E = \frac{9BG}{3B + G} \quad (15)$$

$$\nu = \frac{(3B - 2G)}{2 \times (3B + G)} \quad (16)$$

The elastic properties parameters of the MgZn₂ and T phase calculated in this work were shown in Table 4.

Table 4. Bulk modulus B (GPa), Shear modulus G (GPa), Young's modulus E (GPa), Poisson's ratio ν and B/G of MgZn₂ and T phase.

Phase	Sum	Source	Modulus/MPa		G/B	E	ν
			B	G			
MgZn ₂	Mg ₄ Zn ₈	This work	65.06	32.23	0.49	82.98	0.29
		Ref [24]	64.62	31.71	0.49	81.77	0.29
T phase	Al ₂₆ Zn ₇₂ Mg ₆₄ -C	This work	79.61	37.96	0.47	98.27	0.29
	Al ₂₆ Zn ₇₂ Mg ₆₄ -B		74.69	26.94	0.36	72.15	0.33
	Al ₅₀ Zn ₄₈ Mg ₆₄ -F		80.69	31.58	0.39	83.81	0.32
	Al ₅₀ Zn ₄₈ Mg ₆₄ -BC		73.71	28.97	0.39	76.83	0.32

Poisson's ratio (ν) was the elastic constant of the transverse deformation of the material, reflecting the lateral shrinkage capacity of the material. In the range of 0 to 0.5, the

smaller Poisson's ratio, the harder the material, the smaller the toughness. The ratio of bulk modulus to shear modulus (G/B) can predict the brittleness and toughness of polycrystalline materials. It usually took the value of 0.57 as the critical point of the brittleness and toughness. Metal materials were usually less than 0.57 with good toughness, and the value G/B of the material decreased with the increase of toughness. Table 4 showed that both T phase and $MgZn_2$ phase had good toughness as illustrated by the parameters of G/B and ν .

As for T phase, $Al_{26}Zn_{72}Mg_{64}$ -C phase obtained the highest value of E among the different occupation of Al, Zn atoms, and the value of Young's modulus E of $Al_{26}Zn_{72}Mg_{64}$ -C was higher than that of $MgZn_2$ phase, indicating that $Al_{26}Zn_{72}Mg_{64}$ -C phase gained higher stiffness. It should be noted that the Young's modulus E of $Al_{50}Zn_{48}Mg_{64}$ -F phase was slightly higher than that of $MgZn_2$ phase, while T phase with the other atoms occupation gained lower Young's modulus E than $MgZn_2$ phase. It was implied that the properties of aluminum alloy reinforced by T phase depended on the type of T phase structure.

3.3. Electronic Structures

To illustrate the differences between T phase and $MgZn_2$ phase for structural stability and elastic properties, the total and partial DOS of the T phase and $MgZn_2$ phase were calculated in the present work, respectively, and presented in Figure 2. The common feature of T phase and $MgZn_2$ phase was that there were sharp peaks on the DOS of -8 to -7 eV, which was a typical feature of transition metal caused by the Zn 3d state, indicating that the 3d state was relatively localized, the corresponding band was relatively narrow.

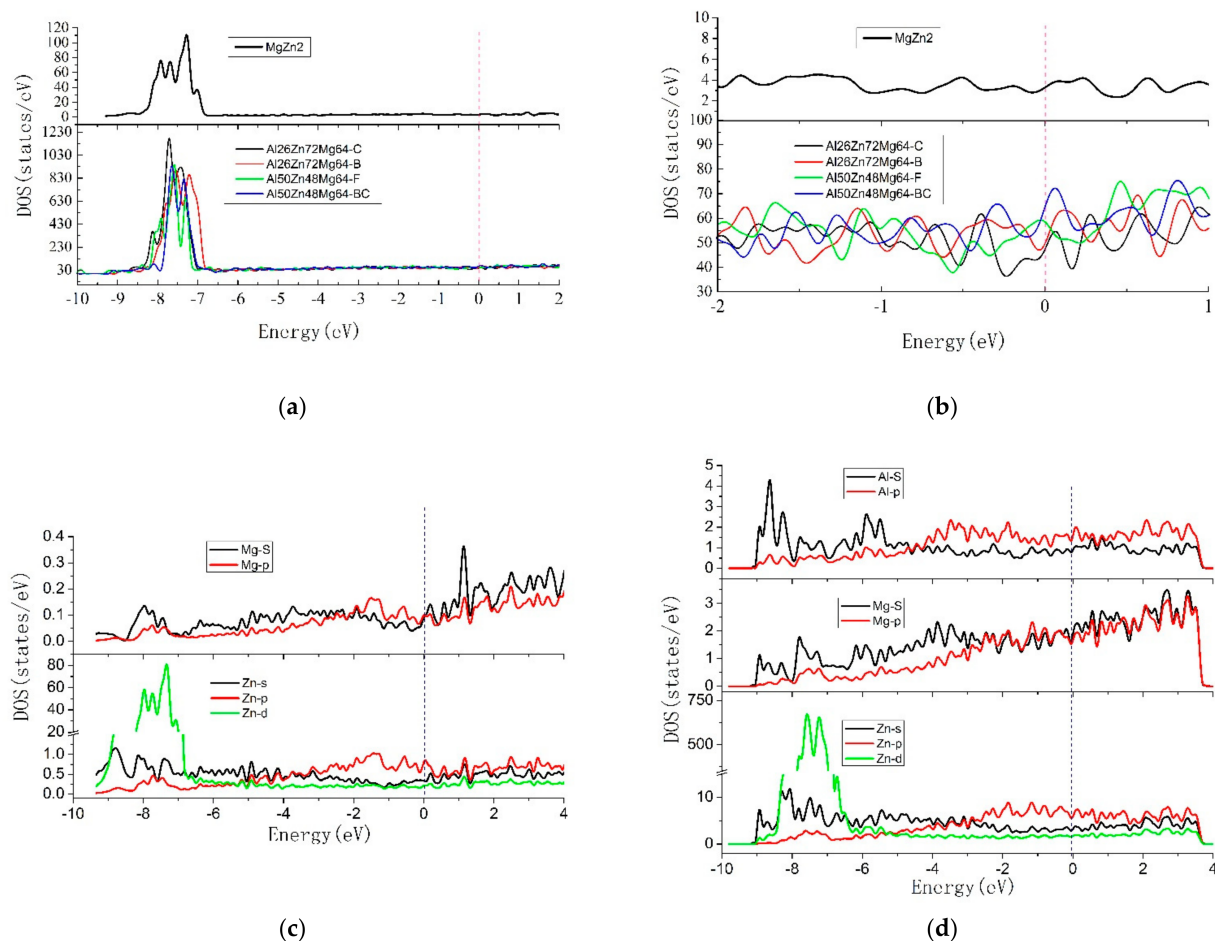


Figure 2. The DOS diagrams: (a) TDOS from -10 to 2 eV of $MgZn_2$ and T-phases; (b) TDOS from -4 to 2 eV of $MgZn_2$ and T-phases; (c) PDOS of $MgZn_2$; (d) PDOS of $Al_{26}Zn_{72}Mg_{64}$ -C.

A larger version of the red dotted line (−2 eV to 1 eV) in Figure 2a was shown in Figure 2b. The Fermi level was set at zero energy and marked by the vertical dotted line in Figure 2b. The inconspicuous gap of DOS located at Fermi energy level, showed that both MgZn_2 phase and T phase mainly presented metallic features, which was mainly controlled by $\text{Mg}3s$, $2p$ and $\text{Al}3s$, $3p$ states.

Electron localization function (ELF) can effectively analyze the degree of electron localization and was used to describe the probability of electron pairs in a multi-electron system to clarify the bonding nature [33]. Compared to DOS, ELF was a suitable tool at determining the nature of the chemical bonding. ELF around these atoms in real space lattice was plotted to reveal the feature of bonding. In Figure 3, ELF = 1 corresponding to the top of the scale with crimson indicates the complete localization, and the middle of the scale with green indicates $\text{ELF} = 1/2$, corresponding to an electron-gas-like type. The calculation results showed that ELF values of MgZn_2 phase was about 0.46 and had the characteristics of electron-gas-like, inferring that the electronic localization was small in MgZn_2 phase, and the interatomic electron mainly presented metal bond. The values of ELF were 0.840, 0.829, 0.857, and 0.844 for $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-C}$, $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-B}$, $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-F}$, and $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-BC}$ phase, respectively. ELF values of T phases were larger than that of MgZn_2 phase, revealing that T phase presented the characteristics of partial covalent bond. As showed in Figure 3, the Al–Zn, Mg–Mg bonding contributed to the high electron localization for $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-C}$ and $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-B}$. As for $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}$, the simultaneous substitution of B, C position by Al atom formed Mg–Zn, Mg–Mg electron localization, while the substitution of F position by Al atom led to the highest electron localization owing to the Al–Al and Mg–Mg bonding. Furthermore, the ELF values of T phase were well-agreed with the higher cohesive energy and phase stability as shown in Table 2.

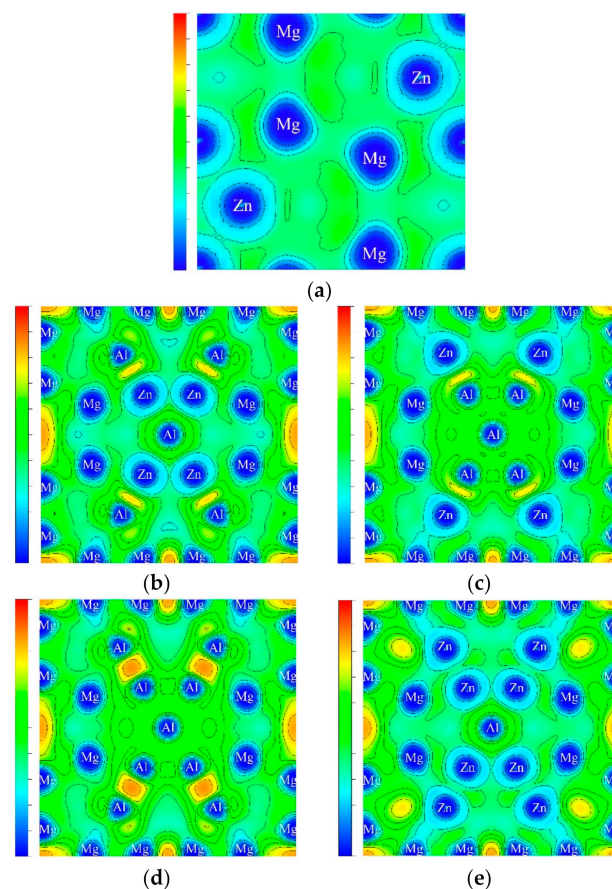


Figure 3. ELF contours: (a) $(11\bar{2}0)$ plane of MgZn_2 ; (b–e) (002) plane of (b) $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-C}$; (c) $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-B}$; (d) $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-F}$; (e) $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-BC}$.

Bader charge can be used to characterize the interatomic ionic bonding. Bader charge calculation results showed that the valence charge of Mg atom in MgZn_2 phase was $-1.43 e^-$ and the valence charge of Zn atom was $+0.67$ and $+0.80 e^-$. The average charge per atom was about $0.95 e^-$, thus there were also ionic bonds between atoms of MgZn_2 phase. Similarly, the average charges per atom of T phase were $1.10e^-$, $0.92e^-$, $0.99e^-$, and $0.93e^-$ for $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-C}$, $\text{Al}_{26}\text{Zn}_{72}\text{Mg}_{64}\text{-B}$, $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-F}$, and $\text{Al}_{50}\text{Zn}_{48}\text{Mg}_{64}\text{-BC}$ phase, respectively. T phase where Al atom respectively occupied the site of C, F had higher Bader charge than MgZn_2 phase, while the Bader charge of T phase was slightly lower than that of MgZn_2 phase when Al atom occupied the site of B and B, C. To a certain extent, the charge transfer indicated the strength of ion interaction, and was positively correlated with Young's E modulus, which was consistent with the mechanical analysis results previously calculated in Table 4.

4. Conclusions

First-principles calculations were applied to explore the cohesive energy, the formation enthalpy, the elastic properties, and the electronic structures of T phase and MgZn_2 phase based on density functional theory. The calculated lattice constants well-agreed with experimental data, revealing the effectiveness of the proposed theoretical models. Al atom in T phase was inclined to occupy the site of C and F in crystal structure. Compared to MgZn_2 phase, T phases obtained lower cohesive energy owing to their partial covalent bond, and revealed that the structural stability of T phase was higher than that of MgZn_2 phase. T phase where Al atom occupied the site of C and F obtained higher elastic modulus, which well-agreed with the calculation of Bader charge per atom.

Author Contributions: B.N. and D.C. conceived and designed the research; Y.S., T.F., F.L. and H.Q. performed the first principles calculation; Y.S. and S.Z. wrote the manuscript. All authors have read and agreed to the published version of the manuscript.

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