The influence of 3d-metal alloy additions on the elastic and thermodynamic properties of $CuPd_3$*

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Embedded-atom method (EAM) potentials are used to investigate the effects of alloying (e.g. 3d-metals) on the trends of elastic and thermodynamic properties for $CuPd_3$ alloy. Our calculated lattice parameter, cohesive energy, and elastic constants of $CuPd_3$ are consistent with the available experimental and theoretical data. The results of elastic constants indicate that all these alloys are mechanically stable. Further mechanical behavior analysis shows that the additions of Cr, Fe, Co, and Ni could improve the hardness of $CuPd_3$ while V could well increase its ductility. Moreover, in order to evaluate the thermodynamic contribution of 3d-metals, the Debye temperature, phonon density of states, and vibrational entropy for CuMPd$_6$ alloy are also investigated.

Keywords: embedded-atom method, lattice inversion, CuMPd$_6$ alloys, elasticity, thermodynamic property

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1. Introduction

Due to their importance in materials science and technological applications, alloys of Pd have been studied both theoretically and experimentally.[1–3] Especially, Pd when alloyed with 3d-transition metals has a strong affect on their structures and hence their physical properties.[4–6] For example, Pd within 5 wt% solute (e.g. V and Cu) forms an ordered phase of 7:1 or 8:1 stoichiometric ratio, which is effective for precipitate hardening.[7] The addition of Mn to Pd crystal induces a diffusionless martensitic transition and shows significant changes in elastic and phonon properties.[8] Previous studies also revealed that Fe–Pd exhibited a competition between the BCC (Pd-poor and low-temperature) structure and the FCC (Pd-rich and/or high-temperature) structure.[9] Further, the Cu–Pd alloy with Pd concentration greater than 50 at% has a disordered FCC structure, while with Pd less than 18 at% it has an $L1_2$-type structure and with 36 at%–46 at% Pd it has an $L1_0$-type structure.[10] It is noteworthy that, in the recent experimental studies, a single phase was formed when $CuPd_3$ was combined with MPd$_3$ (M = 3d metals) at the composition CuMPd$_6$, and their structural, thermal, and magnetic properties have also been investigated.[11] This new ordering behavior in ternary FCC alloy was first presented in $CuMnPt_6$ alloy[12,13] and subsequently aroused wide scientific interest.[14,15]

However, the elastic and vibrational properties focusing on $CuPd_3$ accompany alloying 3d metals have not been studied yet theoretically or experimentally. Therefore, it is of interest to further study these alloys by Chen's lattice inversion embedded-atom method (CLI-EAM). This potential has been applied to Ni–Al intermetallic compounds.[16] Hence, one purpose of this paper is to verify the validity of our alloy potential, while the other aim is to obtain comprehensive data of the physical properties for CuMPd$_6$. Our results are consistent with experimental and theoretical data available in the literature. The present study contributes to the application of Cu–Pd alloys, and may provide general guidance for selecting materials in future experimental work.

2. Details of calculations

2.1. Interatomic potential

In the EAM model, the potential energy of each atom can be represented by[17,18]

$$E = F(\rho_i) + \frac{1}{2}\sum_{i\neq j}\phi(r_{ij}), \tag{1}$$

where $\phi(r_{ij})$ is a pair interaction potential between atoms i and j; $F(\rho_i)$ is the embedding energy as a function of host electron density ρ_i on atom i. The host electron density,

$$\rho_i = \sum_{i\neq j} f(r_{ij}) \tag{2}$$

is the sum of atomic electron densities created at site i by other atoms.

On the basis of Chen's lattice inversion,[19,20] we developed the CLI-EAM potential.[21] The atomic electron density and pair potential function can be expressed, respectively, as

$$f(r) = \sum_n I(n)\rho[b(n)r], \tag{3}$$

$$\phi(r) = 2\sum_n I(n)\{E[b(n)r] - F(\rho[b(n)r])\}, \tag{4}$$

where $b(n)$ is the ratio of the n-th neighbor distance to the first neighbor distance, $r(n)$ is the number of the n-th neighbor

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atoms, $I(n)$ is the inversion coefficient depending only on the structure, which can be written as

$$\sum_{b(n)|b(l)} I(n) r\left(b^{-1}\left[\frac{b(l)}{b(n)}\right]\right) = \delta_{l1}. \quad (5)$$

In this paper, the pair potential is described by the generalized Morse-type function,[22] the embedding function takes the form defined by Banerjea and Smith,[23] the functions of atomic electron density and host electron density each have an exponentially decrease form

$$\phi(r) = D_0\{\exp[-2\alpha(r-R_0)] - 2\exp[-\alpha(r-R_0)]\}, \quad (6)$$

$$F(\rho) = -F_0[1 - n\ln(\rho/\rho_e)](\rho/\rho_e)^n, \quad (7)$$

$$\rho(r) = \rho_e \exp[-\lambda(r/r_{1e}) - 1], \quad (8)$$

$$f(r) = f_e \exp[-\beta(r/r_{1e}) - 1]. \quad (9)$$

The parameters of pair potential between different atoms are acquired by geometrical averaging[18,24]

$$D_{0ij} = \sqrt{D_{0i}D_{0j}}, \ \alpha_{ij} = \sqrt{\alpha_i\alpha_j}, \ R_{0ij} = \sqrt{R_{0i}R_{0j}}. \quad (10)$$

All the input parameters for calculations are listed in Tables 1 and 2.

Table 1. Calculated parameters of pure metal CLI-EAM.

	ρ_e/Å^{-3}	λ	f_e/Å^{-3}	β	n	F_0	D_0	α	R_0
Sc	0.0205	6.002	0.00090	6.303	0.48	2.75	0.149	1.347	3.475
Ti	0.0276	6.077	0.00321	5.232	0.99	2.21	0.252	1.012	3.547
V	0.0385	5.689	0.00340	5.083	0.76	4.54	0.111	2.026	2.744
Cr	0.0434	5.947	0.00396	5.426	0.64	1.35	0.331	1.582	2.792
Mn	0.0392	6.093	0.00304	5.746	0.51	1.70	0.109	1.233	3.005
Fe	0.0326	6.614	0.00308	6.184	0.65	2.75	0.194	1.760	2.682
Co	0.0162	6.284	0.00128	6.250	0.56	3.04	0.227	2.150	2.477
Ni	0.0325	6.355	0.00249	6.181	0.67	2.58	0.220	1.713	2.648
Cu	0.0263	7.044	0.00210	6.814	0.61	1.83	0.190	1.619	2.729
Zn	0.0199	6.236	0.00200	5.512	0.49	0.53	0.123	2.209	2.857
Pd	0.0180	8.038	0.00146	7.889	0.64	1.87	0.268	1.802	2.849

Table 2. Calculated parameters of alloy CLI-EAM.

	Cu–Pd	Sc–Pd	Ti–Pd	V–Pd	Cr–Pd	Mn–Pd	Fe–Pd	Co–Pd	Ni–Pd	Zn–Pd
D_0	0.225	0.200	0.260	0.172	0.298	0.171	0.228	0.246	0.243	0.181
α	1.708	1.558	1.350	1.911	1.688	1.491	1.781	1.968	1.757	1.995
R_0	2.788	3.146	3.179	2.796	2.820	2.926	2.764	2.656	2.747	2.853
	Sc–Cu	Ti–Cu	V–Cu	Cr–Cu	Mn–Cu	Fe–Cu	Co–Cu	Ni–Cu	Zn–Cu	
D_0	0.168	0.218	0.145	0.251	0.144	0.192	0.207	0.204	0.153	
α	1.477	1.280	1.811	1.601	1.413	1.689	1.866	1.665	1.891	
R_0	3.079	3.111	2.736	2.760	2.864	2.705	2.599	2.688	2.792	

2.2. Model

The model of a $2\times2\times2$ supercell with 32 atoms is used to calculate the physical properties of CuMPd$_6$ alloys (Fig. 1). The Cu and M atoms are at the equivalent corner positions while Pd atoms are at the face-centered positions. Defects are not considered, as the major interest is the effect of alloying on the trends of elastic and thermodynamic properties.

2.3. Elastic and thermodynamic properties

According to Ref. [25] by Wallace, the internal energy of a crystal under strain can be expanded by the strain tensor with respect to the energy of the unstrained crystal

$$E(V,\varepsilon) = E(V_0) + \sum_{\alpha:1}^{6}\sigma_\alpha\varepsilon_\alpha + \sum_{\alpha\beta:1}^{6} C_{\alpha\beta}\varepsilon_\alpha\xi_\alpha\varepsilon_\beta\xi_\beta + \cdots, \quad (11)$$

where σ is the stress, ε is the strain, C is the elastic constant, ζ is the factor related to the Voigt index, V_0 and V are the unit cell volumes before and after the deformation, respectively.

Therefore, the second-order elastic constants can be determined from the strain second derivatives of the total energy

$$C_{\alpha\beta} = \frac{1}{V_0}\frac{\partial^2 E}{\partial\varepsilon_\alpha\partial\varepsilon_\beta}\bigg|_0. \quad (12)$$

Since C_{11}, C_{12}, and C_{44} are a complete set of elastic constants for a cubic system, the corresponding mechanical stability conditions are as follows:[25]

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

and the bulk modulus (B), shear modulus (G), Young's modulus (Y), and Poisson's modulus (ν) can be calculated from the following relations:[26,27]

$$B = \frac{1}{3}(C_{11} + 2C_{12}), \quad (14)$$

$$G = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}), \tag{15}$$

$$Y = \frac{9BG}{3B+G}, \tag{16}$$

$$\nu = \frac{3B-2G}{2(3B+G)}. \tag{17}$$

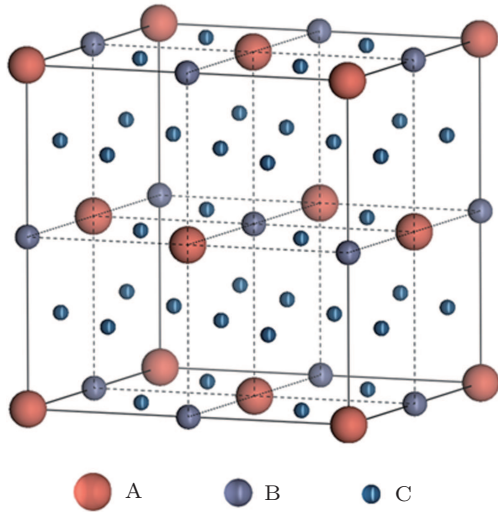


Fig. 1. (color online) The atomic arrangement of an ABC_6-type structure. A, B, and C correspond to Cu, *M* (e.g. 3d-metals), and Pd atoms.

As the vibrational excitations arise solely from the acoustic vibrations at low temperature, we have estimated the Debye temperature from the average sound velocity v_m[27]

$$\theta_D = \frac{h}{k_B}\left[\frac{3m}{4\pi}\left(\frac{N_A\rho_v}{M}\right)\right]^{1/3} v_m, \tag{18}$$

where h and k_B are the Planck and Boltzmann constants, respectively; m is the number of atoms per formula unit; N_A is the Avogadro number; M is the molecular mass per formula unit; $\rho_v(=M/V)$ is the density; and v_m is obtained from[27]

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_s^3} + \frac{1}{v_l^3}\right)\right]^{-1/3}, \tag{19}$$

where the shear (v_s) and the longitudinal (v_l) sound velocities are defined as[28]

$$v_s = \sqrt{G/\rho_v}, \quad v_l = \sqrt{\left(B + \frac{4}{3}G\right)/\rho_v}. \tag{20}$$

The lattice specific heat $C_v(T)$ and vibrational entropy $S(T)$ are derived from the phonon density of states (DOS)

$$C_v(T) = 3Nk_B \int_0^\infty \frac{(\hbar\omega/k_BT)^2 e^{\hbar\omega/k_BT}}{(e^{\hbar\omega/k_BT}-1)^2} g(\omega)\,d\omega, \tag{21}$$

$$S(T) = \int_0^T \frac{C_v(T')}{T'}\,dT'. \tag{22}$$

The entropy difference is calculated by using the following relation:[29]

$$\Delta S_{vib} = S_{vib}^{tot} - S_{vib}^{avg}, \tag{23}$$

where S_{vib}^{tot} is the vibrational entropy of the alloy, and S_{vib}^{avg} is the average of the chemically unmixed state of pure metal weighted by the atomic ratio of alloy.

3. Results and discussion

3.1. Lattice constants and cohesive energies

CLI-EAM alloy potentials are used to investigate the lattice parameters and cohesive energies of CuMPd$_6$ alloys. From Table 3, our calculated lattice constants are in good agreement with theoretical[5,6,30] and experimental[11] results, which suggests that our potential can well describe these Pd-based alloys with acceptable differences. Fleischer[31] suggested that the changes in lattice parameter lead to solute-solution strengthening though interface dislocations. We use a parameter η, which is defined as $(a-a_0)/a_0$, to describe the lattice constant dilation or shrinkage, where a_0 and a are the lattice constants of $CuPd_3$ and CuMPd$_6$, respectively. From Table 3, Sc, Ti, and Zn increase the lattice constants of $CuPd_3$ by 1.5%–3.2%, while other alloying elements do not produce a significant effect on the change of lattice parameter. The obtained cohesive energy of $CuPd_3$ is also consistent with the quantum Sutton–Chen (Q-SC) potential calculation.[6] It is known that the cohesive energy can be used to describe the stability of crystal,[32] and the cohesive energy is often defined as the total energy released by isolated atoms combined into solid. Hence, the larger the absolute value, the more stable the crystal structure is. In Table 3, one can notice that $CuZnPd_6$ has the lowest absolute value of cohesive energy, which means that this alloy is less stable in the ordered structure than other alloys. It may be provide a general guidance for selecting materials in future experimental work.

Table 3. Calculated values of lattice parameter (a), lattice change ratio (η), and cohesive energy (E_c).

	a/Å	η/%	E_c/(kJ/mol)
$CuPd_3$	3.836 (3.834[a], 3.84[b], 3.839[c])		–362.3 (–358.9[b])
$CuScPd_6$	3.958	3.18	–358.9
$CuTiPd_6$	3.939 (3.859[d])	2.68	–372.5
$CuVPd_6$	3.843 (3.846[d])	0.18	–377.1
$CuCrPd_6$	3.853	0.44	–368.8
$CuMnPd_6$	3.861 (3.866[d])	0.65	–352.7
$CuFePd_6$	3.832 (3.845[d])	–0.10	–371.5
$CuCoPd_6$	3.821	–0.39	–375.9
$CuNiPd_6$	3.822	–0.36	–377.4
$CuZnPd_6$	3.892	1.46	–334.2

[a] Ref. [5]; [b] Ref. [6]; [c] Ref. [30]; [d] Ref. [11].

3.2. Elastic properties

As is well known, the elastic modulus can be used to evaluate various fundamental properties, such as bonding characteristic, structural stability, brittleness or ductility, hardness,

strength, and so on.[26,33,34] However, as far as we know, neither theoretically calculated nor experimentally measured values for these properties for CuMPd$_6$ alloys are available. In this section, the calculated elastic constants of CuMPd$_6$ (M = 3d metals) alloys at temperature 0 K are listed in Tables 4 and 5. The elastic constants predicted by the Q-SC potential for the pure $CuPd_3$ at temperature 300 K are also presented and these quantities decrease linearly with temperature increasing.[6] Hence, our results are little larger than these theoretical calculations. It can be seen from Table 4 that the values of our calculated elastic constants satisfy the mechanical stability restrictions (i.e., Eq. (3)), which means that all of the CuMPd$_6$ alloys discussed in this paper have elastically stable structures.

Table 4. Calculated values of elastic constant (C_{ij}), bulk modulus (B), shear modulus (G), Young's modulus (Y), ratio B/G, Poisson's ratio (ν), and the Cauchy pressure (C_{12}–C_{44}).

	Elastic constants/GPa			Modulus/GPa			B/G	ν	C_{12}–C_{44}
	C_{11}	C_{12}	C_{44}	B	G	Y			
$CuPd_3$	207.9	152.3	95.8	170.8	68.6	181.5	2.490	0.323	56.5
	190.4[a)]	132.9[a)]	77.1[a)]	152.1[a)]					55.8[a)]
$CuScPd_6$	178.7	131.3	82.7	147.1	59.1	156.4	2.489	0.323	48.6
$CuTiPd_6$	179.6	134.1	84.2	149.3	59.6	157.8	2.504	0.324	49.9
$CuVPd_6$	212.1	157.1	93.7	175.4	67.2	178.8	2.610	0.330	63.4
$CuCrPd_6$	207.3	149.7	99.4	168.9	71.2	187.2	2.374	0.315	50.3
$CuMnPd_6$	187.0	138.1	86.9	154.4	61.9	163.9	2.494	0.323	51.2
$CuFePd_6$	213.4	156.7	97.1	175.6	69.6	184.4	2.523	0.325	59.6
$CuCoPd_6$	215.7	156.7	98.6	176.4	71.0	187.7	2.485	0.323	58.1
$CuNiPd_6$	218.0	160.3	99.0	179.5	70.9	188.1	2.531	0.325	61.3
$CuZnPd_6$	188.2	133.6	90.5	151.8	65.2	171.1	2.328	0.312	43.1

[a)] Ref. [6].

Table 5. Calculated values of density (ρ_v), Debye temperature (θ_D), and sound velocity (v_s, v_l, v_m).

	ρ_v/(g/cm^3)	v_s/(m/s)	v_l/(m/s)	v_m/(m/s)	θ_D/K
$CuPd_3$	11.26 (11.22[a)])	2468	4826	2765	316
$CuScPd_6$	10.00	2431	4752	2723	302
$CuTiPd_6$	10.19	2419	4739	2711	302 (320[b)])
$CuVPd_6$	11.02	2470	4905	2770	316 (347[b)])
$CuCrPd_6$	10.94	2550	4909	2854	324
$CuMnPd_6$	10.92	2381	4658	2667	304 (311[b)])
$CuFePd_6$	11.18	2495	4900	2796	320 (320[b)])
$CuCoPd_6$	11.32	2504	4892	2805	322
$CuNiPd_6$	11.31	2505	4924	2807	322
$CuZnPd_6$	10.80	2457	4701	2749	310

[a)] Ref. [6]; [b)] Ref. [11].

In order to better reveal the trends of the alloying effects, C_{11}, C_{12}, and B are plotted together in Fig. 2(a). For easy analysis, the x axis in Fig. 2 is arranged in such a way that the atomic number of alloying element presents an increasing order for Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Zn. Figure 2(a) shows that C_{11}, C_{12}, and B follow the same trend as alloying additions. Gschneidner[35] suggested that bulk modulus could be used as a measure of the average atomic bond strength due to its strong correlation with the cohesive energy or binding energy of atoms in crystals. Therefore, Fig. 2(a) indicates that alloying elements Sc, Ti, Cr, Mn, and Zn reduce the average bond strength of $CuPd_3$, while V, Fe, Co, and Ni increase the bond strength.

Figure 2(b) shows the elastic constant C_{44}, shear modulus G, and Young's modulus Y against alloying addition. Haines *et al.*[36] proved that the hardness of a material is closely related to its shear modulus and Young's modulus. We consider that the larger value of the modulus implies the higher hardness of the material. It was also reported that a larger value of C_{44} means higher hardness.[34] From Fig. 2(b) we can see that the alloying elements Sc, Ti, V, Mn, and Zn reduce the hardness of $CuPd_3$ while Cr, Fe, Co, and Ni increase the hardness.

The effects of alloying additions on elastic modulus ratio B/G, Poisson's ratio ν, and Cauchy pressure (C_{12}–C_{44}) are depicted in Fig. 2(c). For the elastic modulus ratio, Pugh[37] suggested that it could be used to describe the plastic properties of metal by considering that the shear modulus represents the resistance to plastic deformation, while the bulk modulus represents the resistance to fracture. A high B/G value is associated with ductility and a low one indicates brittleness, while the critical value is about 1.75.[38] In Fig. 2(c) all the values of B/G are around 2.5, indicating that the doped $CuPd_3$ alloy exhibits a fine ductility. For Poisson's ratio, due to the lack of a direct link between elastic properties and plastic deformation behavior, it is generally accepted that materials with a low Poisson's ratio are brittle.[39,40] Therefore, the alloying elements Cr and Zn significantly increase the brittleness of $CuPd_3$, while V can well improve the ductility of $CuPd_3$. For Cauchy pressure, it is suggested that a positive value indicates ductile behavior, while a negative value means brittle behavior.[41] Further analysis of Fig. 2(c) shows that (C_{12}–C_{44}) has a similar trend to B/G and ν. The difference between (C_{12}–C_{44}) and B/G or ν is that Sc, Ti, and Mn induce a sharp drop in (C_{12}–C_{44}). However, these differences do not produce significant effects

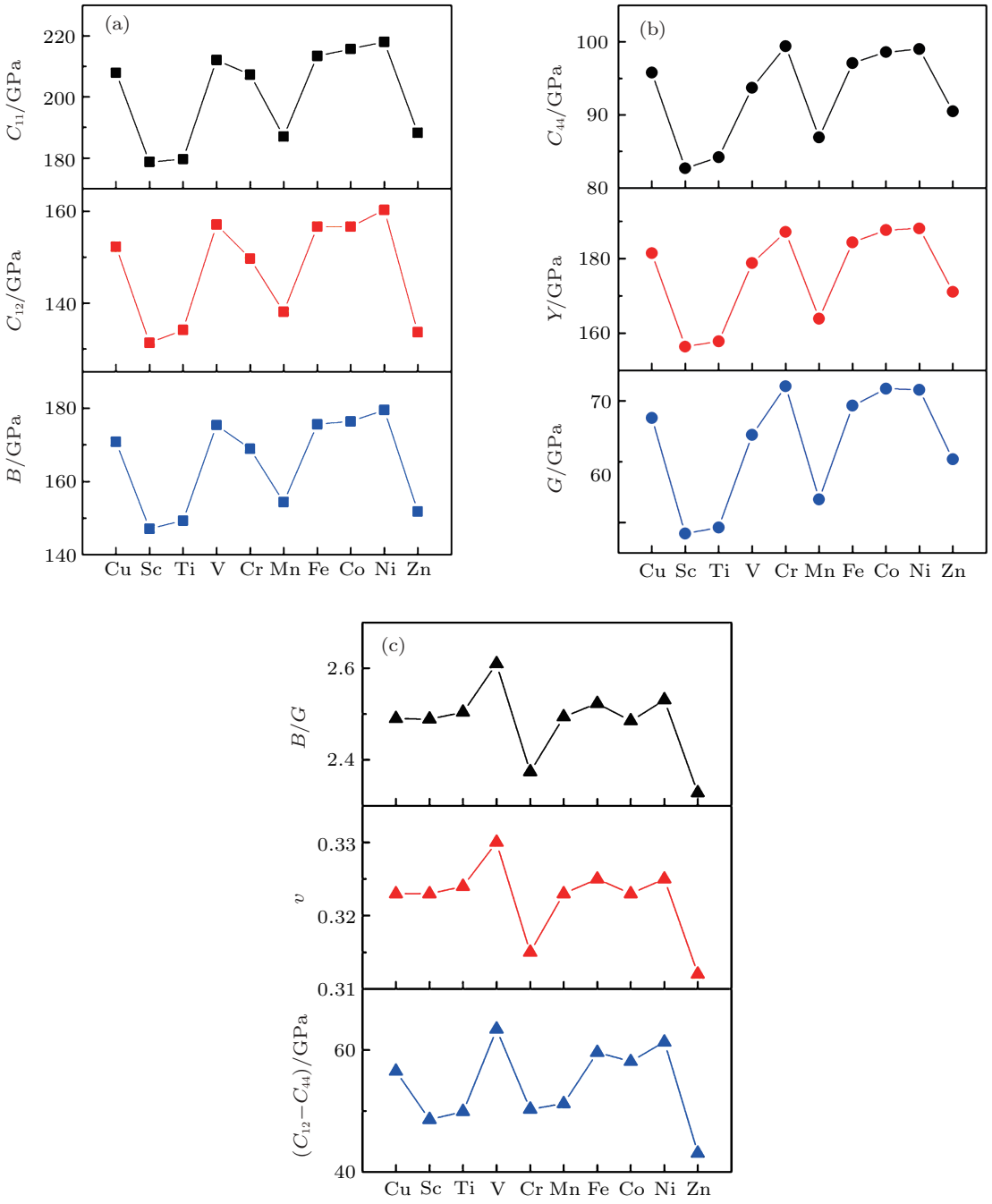


Fig. 2. (color online) (a) Calculated elastic constants C_{11}, C_{12}, and bulk modulus (B) versus alloying addition. (b) The calculated elastic constants C_{44}, Young's modulus (Y), and shear modulus (G) versus alloying addition. (c) The calculated elastic modulus ratio B/G, Poisson's ratio v, and Cauchy pressure (C_{12}–C_{44}) versus alloying additions.

on evaluating the ductile and brittle behavior of doped $CuPd_3$ alloy. In summary, understanding these properties is helpful to assess the mechanical behaviors of materials and be used as a general guidance for selecting materials in future experimental work.

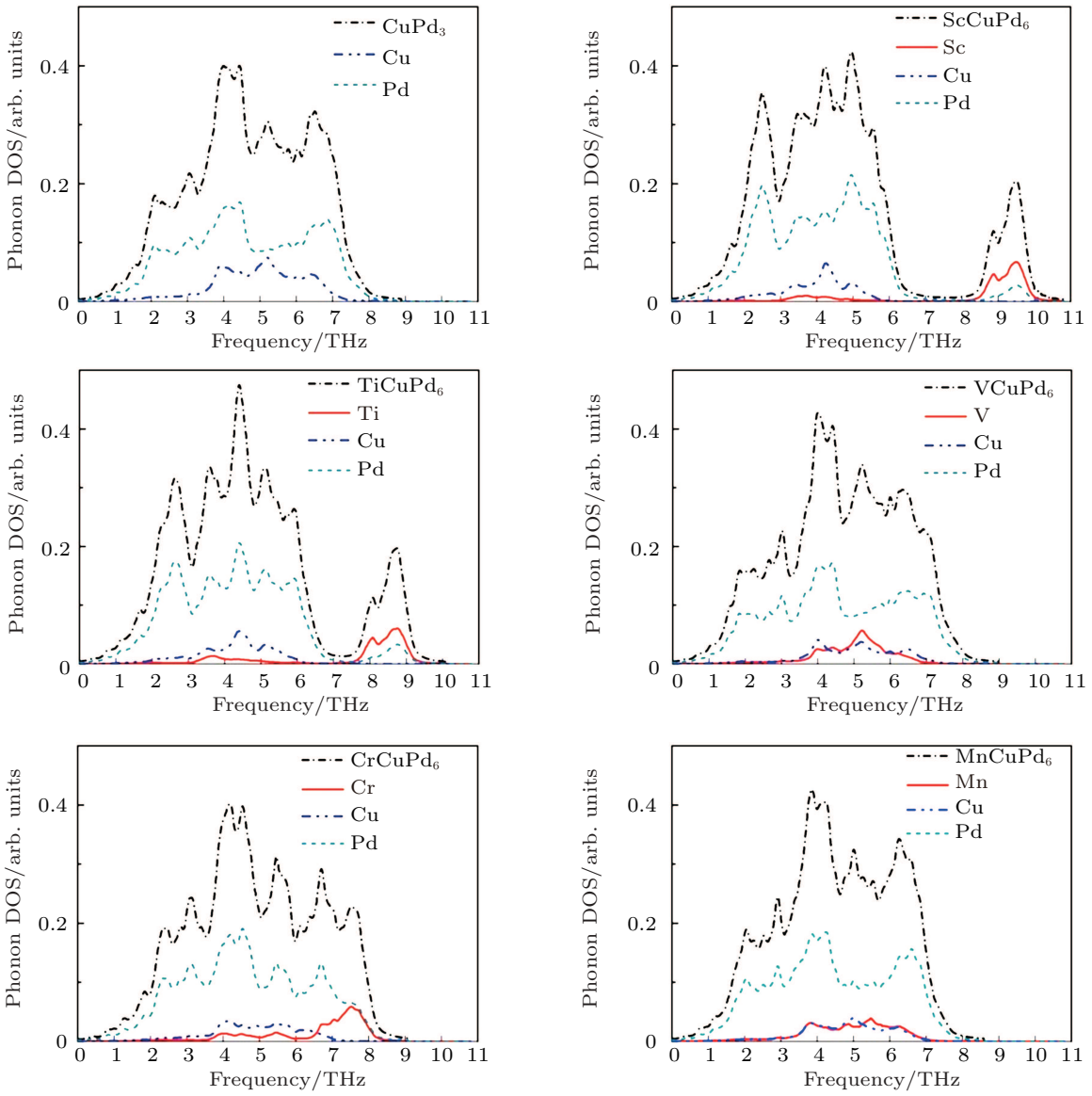
3.3. Thermodynamic properties

In order to gain an insight into the lattice vibrational properties of the new ternary alloys CuMPd$_6$ (M = 3d metals), we calculate their Debye temperatures, phonon densities of states, values of specific heat, and vibrational entropy of these alloys based on the CLI-EAM potential and lattice dynamics theory.

The calculated values of Debye temperature and sound velocity as well as the density for CuMPd$_6$ alloys are list in Table 5. As can be seen, the results are close to the available experimental results[11] and other theoretical[6] calculations. The Debye temperature of $CuPd_3$ is 316 K, while those of other CuMPd$_6$ alloys range from 302 K–324 K, which means that the alloying additions do not produce any significant effect on the Debye temperature of $CuPd_3$ alloy. The probable reasons may be that these specimens are the same in both structure and

major composition, and that their elastic constants, which directly relate to the Debye temperature, have little difference. As is well known θ_D can be used to describe the hardness of material, and its larger value means higher hardness.[42] Further analysis reveals that the alloying elements Sc, Ti, V, Mn, and Zn reduce the value of θ_D, while Cr, Fe, Co, and Ni increase the value of θ_D. The results are consistent with the observed trends of shear modulus and Young's modulus as shown in Fig. 2(b).

The phonon density of state (DOS) reflects the lattice dynamic properties, which is a key quantity for understanding some important thermodynamic parameters. We calculate the total DOSs, as well as the partial DOSs for different alloying elements in doped $CuPd_3$ alloys. The results are displayed in Fig. 3. It can be seen that there are three apexes for $CuPd_3$ around 4.42, 5.2, and 6.70 THz, respectively. While the higher and lower frequency localized modes are mainly contributed by the Pd atoms, and the Cu atoms contribute a major part to the middle frequency modes. The contribution of alloying elements to frequency modes is similar to that of Cu in manner but with a different excited frequency. The detailed information about the excited frequencies for Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn are around 9.52, 8.75, 5.22, 7.52, 5.45 5.35, 5.30, 5.28, 5.20, and 7.00 THz, respectively. Further analysis reveals that with the increase of mass of alloying element, the relevant excited frequencies present a decreasing order, except for V and Zn. The reason may be a strong interaction for V due to the highest bonding energy (5.31 eV[43]) in these alloying elements, while Zn has the lowest bond energy (1.35 eV[43]). In summary, we conclude that an atom is harder to be excited to higher frequency due to its lager mass and stronger interaction. In addition, the alloying elements V, Fe, Co, Mn, and Ni have little effects on the vibrational modes of $CuPd_3$ alloy, while Sc, Ti, Cr, and Zn excite high and low frequency localized modes, with Sc achieving a maximal effect.



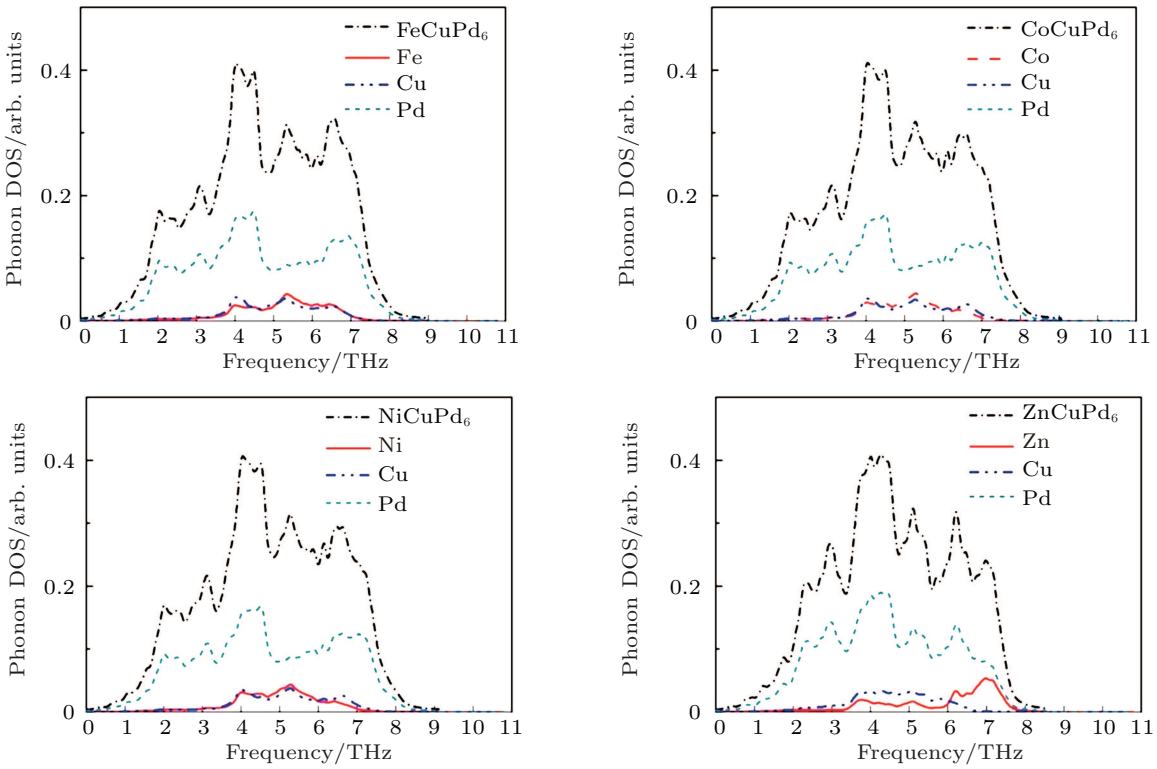


Fig. 3. (color online) The phonon DOS for CuMPd$_6$ alloys.

Some recent measurements show that vibrational entropy affects the relative stability of chemically ordered and disordered phases.[44–46] Moreover, Alam *et al.*[29] proved that the vibrational entropy difference can be used as a measure of the degree of disorder for an alloy. The temperature dependences of the vibrational entropy of mixing as well as the differences in lattice specific heat for CuMPd$_6$ alloys are shown in Fig. 4. It is clear that the specific heat curves have similar shapes, while Sc and Ti cause an obviously increase. A relevant reason may be the similar shapes of the phonon DOS curves of these alloys except Sc and Ti addition. Usually, the higher vibrational entropy of mixing indicates stronger disorder.[29] Therefore,Fig. 4 indicates that alloying elements V, Cr, Fe, and Ni reduce the average disorder strength of CuPd$_3$, while Sc, Ti, Co, Mn, and Zn increase the disorder strength, with Sc achieving a maximal effect. Unfortunately, due to the absence of these properties in the literature, the calculated results may be regarded as an attempt to predict the vibrational properties for the ternary alloys. Future experimental work will provide a comparison with our calculated results.

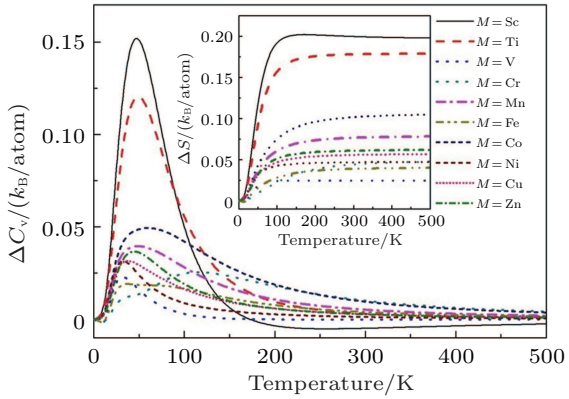


Fig. 4. (color online) The calculated differences in lattice specific heat for CuMPd$_6$ alloys. The inset shows a similar estimate of vibrational entropy of mixing.

4. Conclusions

In this work, a wide range of physical properties for doped CuPd$_3$ alloy are investigated. We find that our alloy potential is an effective method of investigating the properties of CuMPd$_6$ (M = 3d metals) alloys. The results for lattice parameter, cohesive energy, elastic constant, density, and Debye temperature show satisfactory agreement with available experimental results and other theoretical calculations. To our knowledge, the effects of alloying on the elastic and thermodynamic properties of CuMPd$_6$ alloys are presented here for the first time. We use the bulk modulus, shear modulus, Young's modulus, Poisson's ratio, the elastic modulus ratio, and Cauchy pressure (C_{12}–C_{44}) to assess the elastic properties. The results show that alloying with Cr, Fe, Co, and Ni could improve the hardness of CuPd$_3$ alloy. The addition of V could well increase the ductility of CuPd$_3$ alloy, while Zn exerts an opposing effect. For thermodynamic properties, we extensively study the Debye temperature, phonon density of states, and vibrational entropy of mixing. Analyses of the above quantities suggest that the alloying addition does not

produce a significant effect on the thermodynamic property for $CuPd_3$ alloy.

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