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Molecular dynamics study of Cu-Pd ordered alloys

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Analysis and modelling

ABSTRACT

Purpose: The goal of the paper is to study the molecular dynamics of Cu-Pd ordered alloys.
Design/methodology/approach: The thermal and mechanical properties of Cu, Pd pure metals and their ordered intermetallic alloys of $Cu_3Pd(L1_2)$ and $CuPd_3(L1_2)$ are studied by using the molecular dynamics simulation. The melting behavior of the metals considered in this work is studied by utilizing quantum Sutton-Chen (Q-SC) many-body potential. The effects of temperature and concentration on the physical properties of Cu-Pd system are analyzed.
Findings: A wide range of properties of Cu, Pd pure metals and their Cu_3Pd and $CuPd_3$ ordered intermetallics is presented. It was found that this potential is suitable to give the general characteristics of the melting process in these systems.
Practical implications: The simulation results such as cohesive energy, density, elastic constants, bulk modulus, heat capacity, thermal expansion and melting points are in good agreement with the available experimental data and other theoretical calculations.
Originality/value: To the best our knowledge this work presents, for the first time, a wide range of physical properties of alloys focusing on Cu-Pd ordered compounds.
Keywords: Cu-based intermetallic alloys; Molecular dynamics simulations; Quantum Sutton-Chen potentials; Melting properties

1. Introduction

With the rapid development of advanced technologies, the demands for the design of components and the production of new materials which are strong, stiff and ductile at high temperature and the study of the final product properties are increasing. Stable materials responding these requirements are the intermetallic compounds. They have structural properties which differ greatly from constituent metals.

Cu-based intermetallics have motivated the strong interest in their fundamental properties including interatomic bonding, long range order, crystalline defects, order-disorder transition and diffusion [1-14]. Among them, CuPd has receiving considerable attention due to their promising use as catalysts in many technologically important areas, including petroleum refining and automotive emission control, and membrane for hydrogen production and purification. On the other hand, Cu_3Pd and $CuPd_3$ being ordered alloys of Cu-Pd system offer to be investigated due to a little of theoretical and experimental studies. In fact, relatively attention has been paid to the temperature dependence of the thermodynamical and mechanical properties of the ordered Cu_3Pd and $CuPd_3$ intermetallic compounds. In this work this specific problem is addressed.

Some first principles (*ab initio*) calculations responsible for the physical properties of Cu-Pd system have recently been carried out successfully [1, 2, 11-13]. Because *ab initio* methods are computationally expensive, the calculations have been limited to short time scales and to a few hundred atoms. On the other hand,

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there are empirical and more practical approaches that can afford to investigate many system and trends in physical properties [15-18]. These potentials provide sufficiently accurate and quick description in metallic systems. Molecular dynamics (MD) simulation can provide an important insight by allowing one to determine static and dynamical properties of materials at finite temperatures, when provided with suitable interatomic potentials.

In this study, we have performed MD simulations using Sutton-Chen (SC) [18] potential with new potential parameter set, namely the Quantum Sutton-Chen (Q-SC) potential developed by Çağın and co-workers [19] to investigate the physical properties of Cu and Pd pure metals and ordered Cu-Pd alloys (especially, $Cu_3Pd(L1_2)$and $CuPd_3(L1_2)$). This potential has been used in various applications, ranging from random alloys, glass formation, crystallization, surfaces, clusters, nanowires and single crystal plasticity of pure metals to transport properties of fcc metals [20-26]. One purpose of this study is to verify the validity of potential parameters to show their transferability from pure elements to ordered alloys, from low temperatures to high temperatures. Another aim is to obtain comprehensive data of the physical properties of ordered Cu-Pd, which is scientifically and technologically important material. In this study, we have calculated the lattice parameter, cohesive energy, density, elastic constant and bulk modulus at various temperatures and deduced the melting temperature, heat capacity and thermal coefficient of the volume expansion by using Q-SC potential parameters. The results are compared with experimental and theoretical data available in the literature. To the best our knowledge this work presents, for the first time, a wide range of physical properties of alloys focusing on Cu-Pd ordered compounds.

This paper has the following structure: simulation details are presented in Section 2. Section 3 deals with the results of computer simulations. The final section gives the conclusion of the results.

2. Simulation details

Three successive simulations are performed for heating process of Cu-Pd alloys by using the algorithm based on extended Hamiltonian formalism [27-31]. First, constant-enthalpy constant-pressure (HPN) MD simulation is carried out to heat the system from 0.1 K to 2500 K with the increments of 50 K. This increment is reduced to 10 K near the melting temperature to get more accurate values of the melting temperature. The heating procedure is carried out by scaling velocities with the ratio of the increment temperature to the specific number of steps depending on target temperature, (1 K/step). At each temperature, 2000 time steps are carried out for equilibrium. Then 20000 additional steps in constant-temperature constant-pressure (TPN) dynamics are taken to obtain some statistical properties, such as volume, density and energy of the system. Finally, 50000 steps of microcanonical ensemble (EVN) dynamics follows by using the resulting zero strain average matrix to obtain pressure dependent properties of the system, such as elastic constant.

The simulation box is made up of 2048 particles arranged on the fcc structure for the pure Cu and Pd, $L1_2$ structure for the Cu_3Pd and $CuPd_3$ ordered intermetallic systems. In the case of Cu_3Pd, the Pd atoms occupy the corner cites, while Cu atoms occupy the face centres of the basis cube; the opposite occurs for $CuPd_3$. The MD simulation performed in this study uses the Sutton-Chen (SC) type potential [18]. This potential is recently reparametrized by Çağın *et al.* [19] by including quantum corrections accounting for zero-point energy, hence called quantum Sutton-Chen (Q-SC) potential, to improve some physical properties at high temperatures. The potential parameters are obtained by fitting to some experimental properties, such as lattice parameter, cohesive energy, bulk modulus, phonon frequency at the X point, vacancy formation energy and surface energy. The total potential energy has the following form:

$$U_{tot} = \sum_i^N U_i = \sum_i^N \left[\sum_{j\neq i} \varepsilon_{ij} \frac{1}{2} \left(\frac{a_{ij}}{r_{ij}} \right)^{n_{ij}} - c_i \varepsilon_{ii} \left(\sum_{i\neq j} \left(\frac{a_{ij}}{r_{ij}} \right)^{m_{ij}} \right)^{1/2} \right] \tag{1}$$

The first term in Eq. 1 is a two body repulsive interaction between the atoms *i* and *j*, separated by a distance r_{ij}. The second term represents the many-body cohesion term associated with atom *i*. The square root term introduces a many-body component into the energy summation. The popularity of SC potentials is partly due to the computationally tractable form adopted for the many-body forces. It is the relatively simple analytic form of the potential that enables one to calculate the many physical properties of the materials.

In the Eq. 1, a is a length parameter scaling to the lattice spacing of the crystal, c is a dimensionless parameter scaling the attractive terms, ε is an energy parameter determined from experiment, and n, m are integer parameters with $n < m$ which determine the range of the two components of the potential. The interaction length of potential is taken as two lattice parameters for the efficiency of the computer simulation time. The temperature effects in the simulations are considered by giving an additional length of half the lattice parameter. The parameters for the Cu-Pd alloys are obtained through the following mixing rules [32]:

$$\varepsilon_{ij} = (\varepsilon_i \varepsilon_j)^{1/2}, \qquad a_{ij} = \frac{a_i + a_j}{2},$$
$$m_{ij} = \frac{m_i + m_j}{2}, \qquad n_{ij} = \frac{n_i + n_j}{2} \tag{2}$$

Q-SC potential parameters [19] for pure Cu and Pd metals are given in Table 1.

Table1.
Q-SC potential parameters for Cu and Pd pure metals

Metal	n	m	$\varepsilon(meV)$	c	$a(A^\circ)$
Cu	10	5	5.7921	84.843	3.6030
Pd	12	6	3.2864	148.205	3.8813

The fluctuation formula for the calculation of the elastic constants [33-35] is given as:

$$C_{ijkl} = \frac{V_0}{k_B T} \left(\langle P_{ij} P_{kl} \rangle - \langle P_{ij} \rangle \langle P_{kl} \rangle \right) + \frac{2 N k_B T}{V_0} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) + \langle \aleph_{ijkl} \rangle \tag{3}$$

The first term represents the contribution of the fluctuation of the microscopic stress tensor P_{ij}, the second term is the kinetic energy contribution, and third term is the so-called Born term. <> denotes the averaging over time and $V_0 = \det h_0$ is the reference volume for the model system. The bulk modulus for the cubic systems can be obtained from $B = (C_{11} + 2C_{12})/3$. Specific heat and coefficient of thermal volume expansion can be determined from the differential of the enthalpy and that of volume, respectively, as follows:

$$C_p(T) = \left(\frac{\partial H(T)}{\partial T}\right)_P, \quad (4)$$

$$\alpha_p(T) = -\frac{1}{V(T)}\left(\frac{\partial V(T)}{\partial T}\right)_P. \quad (5)$$

3. Results

Table 2 shows some thermodynamical properties, namely density ρ, lattice constant a, cohesive energy E_c and compressibility κ of CuPd ordered metal alloys calculated from TPN ensemble average over 20000 time steps at 300 K, together with available experimental or theoretical data. The results for Cu and Pd pure metals are in good agreement with the experimental data [36]. The discrepancy between Q-SC and experimental values for the first three properties is less than 1%, for compressibility of Cu 20.5% and for that of Pd 12.5%. We expect that the results of compressibility will be improved at high temperatures because Q-SC potential describes well temperature dependent properties. There is not any experimental data for Cu_3Pd and $CuPd_3$ alloys to compare our results with them. The values of lattice constants calculated for the ordered alloys are close to that of other theoretical studies [10, 37]. The increasing concentration of Pd in Cu-Pd compounds gives rise to decreasing the cohesive energy of the Cu-Pd intermetallics, while it causes an increment in lattice parameter and density, as expected.

We calculated the heat capacity as a function of temperature and concentration by fitting the enthalpy of Cu-Pd alloys to a quadratic polynomial using the data below the melting temperature. The quadratic function form may be given as

$$H(T) = a + bT + cT^2 \text{ (kJ/mole)}. \quad (6)$$

Here T is the temperature. Heat capacity can be found by taking the derivative of the polynomial function of Eq. 6 according to Eq. 4. The resulting C_p should not be extrapolated to T=0 K, as it is derived from $H(T)$ which is fitted to simulation results between 100 K and 700 K. The coefficients of expression in Eq.6 are given in Table 3.

As shown in Table 3, the agreement between the simulated results and experimental data [38] is very good. For example, the heat capacities of Cu and Pd at 300 K are reported as 26.359 $Jmole^{-1}K^{-1}$ and 25.791 $Jmole^{-1}K^{-1}$, respectively. Deviations from the experimental values for Cu and Pd are 7.75 % and 0.73 %, respectively.

We have also fitted the volume and temperature curve by the same type of quadratic polynomial function as done in the heat capacity to analyze further the volume thermal expansion behaviour. The function used in the fitting procedure is

$$V(T) = a + bT + cT^2 \text{ (nm}^3\text{mole}^{-1}\text{)}. \quad (7)$$

The coefficients in Eq.7 and the values of the thermal volume expansion calculated from Eq. 5 at 300 K are presented in Table 4. The value for copper, 7.642×10^{-5} K^{-1}, is in better agreement with the value from the experiment [38] than other experimental value measured by Moruzzi et al. [39]. For palladium, our simulation result is greater than experimental value of 1.160×10^{-5} K^{-1} [39].

Table 2.
Density ρ, lattice constant a, cohesive energy E_c and compressibility κ of CuPd ordered metal alloys calculated by using Q-SC potential parameters at 300 K, together with a comparison with available experimental [36] or theoretical data. Stars correspond to other theoretical results [10, 37]

Material	E_c (kJ/mol)		$a(A^\circ)$		ρ (g/cm^3)		κ (10^{-11}m^2/N)	
	Exp	Q-SC	Exp	Q-SC	Exp	Q-SC	Exp	Q-SC
Cu	-336.0	-339.58	3.61	3.62	8.93	8.93	0.73	0.58
Cu_3Pd		-339.89	3.694*, 3.705**	3.70		9.73		
$CuPd_3$		-358.87	3.839*, 3.834**	3.84		11.22		
Pd	-376.0	-377.91	3.89	3.90	12.00	11.96	0.55	0.62

* from [37], ** from [10]

Table 3.
Coefficients of polynomial function used to find the heat capacity of Cu, Pd pure metals and their alloys. Heat capacity values of the metals along with whenever available experimental data [38] at 300 K

Material	a	$bx10^{-4}$	$cx10^{-6}$	C_p (J/moleK)	
				Q-SC	Exp
Cu	-339.672	249.787	2.300	26.359	24.464
Cu_3Pd	-347.680	255.138	1.609	26.479	
$CuPd_3$	-366.437	244.646	2.247	25.813	
Pd	-377.824	246.235	1.945	25.791	25.980

We calculated the elastic constants of Cu-Pd ordered alloys to study the mechanical and dynamical properties. The elastic constants, in particular, provide valuable information on the stability and stiffness of materials. In this study, elastic constants are calculated by using the fluctuation expression (3) by taking the average ensemble of EVN over the 50000 time steps. The elastic constants and bulk modulus results for Cu and Pd pure metals and their ordered alloys are listed in Table 5. At each temperature, the density obtained from TPN ensemble by averaging over the 20000 time step is used to specify the volume of the EVN ensemble. The detailed calculation methodology related to the elastic constants can be found in Refs. [35]. The elastic constants and bulk modulus of Cu and Pd pure metals predicted from Q-SC parameters are compared with the available experimental values and the results of previous works using different potential models at 0 K in Table 5. As shown, the potential used by Cleri and Rosato [40] for the elastic constants is yielding better results. The elastic constants and bulk modulus from Q-SC agree with the available experiment and other calculations except for elastic constant of C_{12}. The percentage differences of C_{11}, C_{12} and C_{44} of Cu for the Q-SC are 9.8%, 2.9% and 11.1% at 0 K, respectively. The accuracy of the Q-SC elastic constant of C_{11} for Pd, showing a deviation of 8% from experiment, is comparable to that of the embedded atom model (EAM) [41]. The experimental data on the elastic constants for Cu-Pd alloys are not available for comparison.

Table 4.
Coefficients of polynomial function used to find the thermal volume expansion of Cu, Pd pure metals and their alloys. Thermal expansion values of the metals along with whenever available experimental data [38, 39] at 300 K

Material	$ax10^{-4}$	$bx10^{-9}$	$cx10^{-12}$	$\alpha_p x10^{-5}$ (K^{-1}) Q-SC	Exp
Cu	116.023	734.596	281.536	7.642	1.670[1] 4.950[2]
Cu_3Pd	124.252	757.483	232.696	7.090	
$CuPd_3$	139.136	749.161	200.403	6.149	
Pd	145.387	748.575	179.893	5.802	25.980

[1] from [39], [2] from [38]

Table 5.
Comparison of calculated and experimental (Exp) [42] values for elastic constants (C_{ij}) and bulk modulus (B) at 0 K for pure metals in the units of GPa. For Cu-Pd alloys, the elastic constants are predicted from Q-SC potential parameters at 300K. Our results (Q-SC) for Pd and Cu are compared with the other potential models: embedded atom model (EAM) [41] and tight binding second moment approximation (TBSMA) [40, 43]

Metals	Model	C_{11}	C_{12}	C_{44}	B
Cu	Q-SC	159.00	121.30	72.74	127.50
	Exp[1]	176.20	124.94	81.80	142.03
	TBSMA[2]	176.00	125.00	82.00	142.00
	TBSMA[3]	142.00	180.00	122.00	142.00
Cu_3Pd	Q-SC	166.71	117.97	67.85	134.22
$CuPd_3$	Q-SC	190.44	132.90	77.08	152.08
Pd	Q-SC	216.00	150.25	91.66	172.17
	Exp[1]	234.12	176.14	71.17	195.00
	TBSMA[2]	232.00	178.00	73.00	196.00
	EAM[4]	218.00	184.00	65.00	195.00

[1] from [42], [2] from [40], [3] from [43], [4] from [41]

We are also interested in investigating the temperature and concentration dependence of elastic constants of Cu-Pd ordered system to see the effect. The variation of elastic constants of Cu-Pd in the fcc structure for pure metals and in the $L1_2$ structure for Cu_3Pd and $CuPd_3$ ordered alloys as a function of temperature are given in Figure 1a-d, respectively. These quantities decrease linearly with increasing temperature, as seen in the Figures. Thermal softening increases with increasing the concentration of Cu in Cu-Pd system at each temperature.

The melting temperatures of Cu-Pd ordered alloys have been determined by analyzing the behaviour of density, energy, volume and pair distribution function as a function of temperature. We obtain the same melting temperatures from all these physical properties. Computer simulations are carried out by 10 K increments around the melting point in order to make better predictions of the melting point. In this manner, the melting points of the pure elements and intermetallic systems are predicted for Q-SC parameters. The results are listed in Table 6, along with the available experimental [44] and other theoretical data [41, 45, 46]. As shown in the table, the melting points of pure Cu (1370±10 K) and Pd (1820 ±10 K) metals are in very good agreement with experimental values. As we go into the alloy, this accuracy decreases with the maximum deviation of 3.20%. This is due to the potential parameters of binary metal alloys calculated by using those of pure metals using combination rules (Eq. 2). Our result for the melting temperature of Cu are in excellent agreement with the other calculation based on EAM [35].

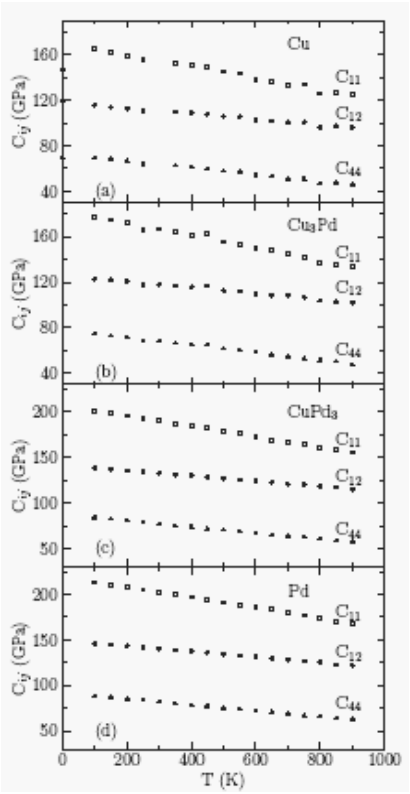

Fig. 1. The variation of elastic constants as a function of temperature for a) Cu, b) Cu_3Pd, c) $CuPd_3$ and d) Pd

Table 6.
Melting points of Cu-Pd ordered alloys and Cu and Pd pure metals along with experimental [44] and other calculation results [41, 45, 46], where available

Mater.	T_m(K)			Devia.
	Q-SC	Exp	Other calculations	(%)
Cu	1370±10	1356	1370[1],1073[2]±17,1340[3]	1.03
Cu_3Pd	1450±10	1405		3.20
$CuPd_3$	1700±10	1650		3.03
Pd	1820±0	1825	1215±20[2],1390[3]	0.27

[1] from [45], [2] from [46], [3] from [41]

The temperature dependence of density, volume and energy of Cu, Pd, Cu_3Pd and $CuPd_3$ are shown in Fig. 2(a), (b) and (c) respectively. The discontinuity in the Figures shows the structural transformation from solid phase to liquid phase. The melting temperature is identified by monitoring the jump in the Figures. At the melting temperatures, we find the density for Pd and Cu to be 10.53±0.06 and 7.64 g/cm^3, respectively. These values are consistent with experimental values which are 10.49 and 8.00, respectively [47].

The way we follow to predict the melting temperatures from the pair distribution function g(r) is observed in Fig. 3 plotted at the selected temperatures; 1600, 1810, 1820 and 2000 K for Pd. The peaks at 1600 K could be one by one related to the different coordination shells of a perfect fcc structure. With increasing temperature up to 1810 K the peaks are broadened and lowered, showing the structure with the peaks at near some of the ideal fcc position. At the temperature of 1820 K some peaks disappear, indicating that a diffusion dynamics is thermally activated. Finally, the crystal order is broken and melting occurs after this temperature. That is, the metal goes into the liquid state (2000 K).

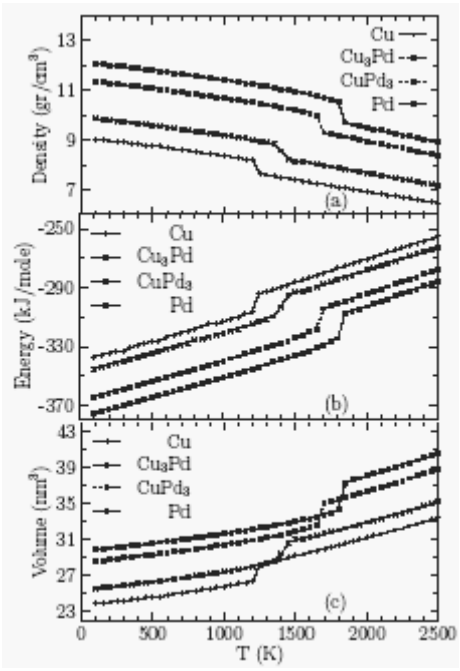

Fig. 2. (a) Density, (b) energy and (c) volume of Cu, Pd , Cu_3Pd and $CuPd_3$ as a function of temperature

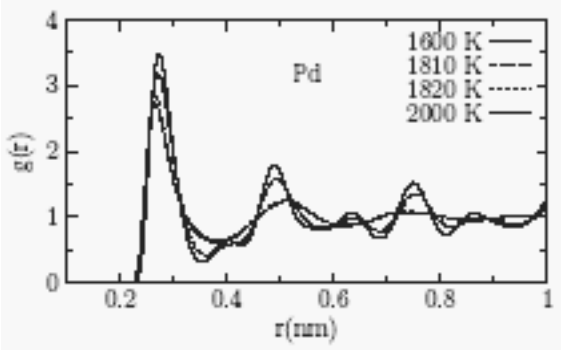

Fig. 3. Pair distribution function g(r) for Pd at various temperatures

4. Conclusions

We have presented a wide range of properties of Cu, Pd pure metals and their Cu_3Pd and $CuPd_3$ ordered intermetallics. We have found that this potential is suitable to give the general characteristics of the melting process in these systems. The transferability of the potential is an important conclusion which can be made from this work. Although the potential parameters were fitted to solid experimental properties of the pure system, the Q-SC model describes the thermal and mechanical properties of the liquid Cu-Pd system. Because the only experimental data for Cu-Pd metal alloys exits for the melting points, we can test the transferability from experimental case to alloy case for melting. That the results for density, lattice constants, cohesive energy, compressibility, elastic constants, heat capacity and thermal expansion coefficients of pure metals show satisfactory agreement with available experimental values leads us to conclude that transferability of the potential is proved for pure metal cases.

To our knowledge, the temperature dependence of physical properties for Cu_3Pd and $CuPd_3$ ordered alloys are presented for the first time, in this study. If the potential energy function considered here is fitted to the solid properties of the intermetallic compounds of Cu_3Pd and $CuPd_3$, the results may be improved further.

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