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MODIFIED MODULATED FIRSTORDERPOLYNOMIAL PAIRPOTENTIAL FUNCTION FOR CALCULATING TEMPERATURE-DEPENDENT PROPERTIES OF BODY CENTERED CUBIC

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ABSTRACT

Potential functions which described the anharmonic oscillators could reasonably predict metallic properties which are temperature dependent at room temperature but failed when applied to calculate these set of parameters at high temperatures. This is why a temperature dependent first order polynomial modulated by a simple exponential pair potential function was developed to estimate temperature-dependent properties of metallic .cubes, such as the coefficient of thermal expansionand the specific heat capacity of some selected cubic metals at temperatures higher thantheroomtemperature.The adjustableparametersin this pair potentialfunctionwere fitted to the lattice constant,the internal energy and the bulk modulusof the cubic consider in this study. The results generated showed a good agreement with both experimental values and some theoretical values of thermalcoefficients and elastic constants found in literature.

KEYWORDS: Coefficient of.Thermal Expansion (CTE), Lattice Constants, Modulated Pair Potential, Anharmonic Oscillator, Low and High Temperatures.

1.0INTRODUCTION

A modulated first order pair potential function is developed to analyze some of the temperature dependent parameters of some selected metallic cubic. In a cubic metal, the atoms arrange themselves ina regular pattern so that the potential energyofthesystem is at minimum. Theyare rigidly fixed but vibrate about their respective equilibrium position with

amplitude that goes on increasingwithrise in temperaturewhich expresses the thermalexpansionof metals. The thermal expansion of metals can be qualitatively explained as a result in displacement of equilibrium position of the atoms due to increase of the amplitude of vibration FA. Hummel (1950). Since temperature is the physical quantity that implies atomic vibration, resulting in the anharmonic vibration, it also causes the phenomenon of thermal expansion which is a temperature dependent behavior. In view of the influence of atomic vibration on thermal expansion of metals, attempts were made by several workers to correlate this property vibration characteristics of the atoms. Some potentials due to Morse potential Girifalco and Weizer (1959) and Daw and Baskes (1984) embedded atom method EAM proposed to estimate the thermal expansion ofmetals at room temperature. Davis (1990)metals hand book, Foiles S.M., DawM.S (1988) calculation of thermal expansion of metals using embedded atom method. Another well-known model for thermal expansion calculation was developed by Moruzzi et al.

Withallthis,noonehaseverusedthismodulatedfirstorderpairpotentialfunctionin determiningthetemperaturedependentthermalexpansionofmetals.Usingmodulatedfirstorder, polynomial pair potential function, the thermal expansion coefficient of some cubic metals were calculated.Thetemperaturedependentthermalexpansionofmetalswasalsoexpressedin

graphical representation. The parameters of the modulated pair potential function were obtained by fitting lattice constants and bulk modulus. This method yield CTE in good agreement with experimental value and also expressed temperature dependent thermal expansion of cubic metals.

11 THEORY

A modulated first order polynomial pair potential, of the form

$$\phi(r_{ij}) = \phi_e\left\{1+\beta\left(\frac{r_{ij}}{r_e}-1\right)\right\}\exp\left(-\alpha\left(\frac{r_{ij}}{r_e}-1\right)\right) \quad \text{..... (1)}$$

is used in this study to represent the interaction between two atoms in metallic cube. In this expression there are three adjustable parameters, (α, β and ϕ_e). The parameter r_e is the equilibrium interatomic distance. It is equally used to determine the cut off distance of the potential function which lies within the first nearest neighbour atoms. The parameter r_{ij} defines the atomic distance between atoms i and j.

The total energy, $E(rij)$ of a metallic system is obtained by summing equation (1) over the entire atoms within this metallic cube, thus the average energy of the system is given as;

$$E(rij) = -\frac{N\phi_e}{2}\sum_j\left\{1+\beta\left(\frac{r_j}{r_e}-1\right)\right\}\exp\left(-\alpha\left(\frac{r_j}{r_e}-1\right)\right) \quad \text{..... (2)}$$

where N is the Avogadro's number.

This energy equation written in a molecular framework concept can be rewritten as;

$$E(a) = P\sum_j\left\{1+\beta\left(\frac{M_j a}{r_e}-1\right)\right\}\exp\left(-\alpha\left(\frac{M_j a}{r_e}-1\right)\right) \quad \text{..... (3)}$$

where $P = -\frac{N\phi_e}{2}$; $r_j = \left[m_j^2+n_j^2+l_j^2\right]^{1/2}$ $a = M_j a$ and a is the lattice constant.

The first and the second derivatives of the energy of equation with respect to the lattice constant a are given by

$$\frac{dE(a)}{da} = P\sum_j\left\{\frac{\beta M_j}{r_e}\exp\left(-\alpha\left(\frac{M_j a}{r_e}-1\right)\right)+\left[1+\beta\left(\frac{M_j a}{r_e}-1\right)\right]\left(\frac{\alpha M_j}{r_e}\right)\exp\left(-\alpha\left(\frac{M_j a}{r_e}-1\right)\right)\right\} \quad \text{.....(4)}$$

$$\frac{d^2E(a)}{da^2} = P\sum_j\left\{\frac{-\alpha\beta M_j^2}{r_e^2}\exp\left(-\alpha\left(\frac{M_j a}{r_e}-1\right)\right)+\left[\left[1+\beta\left(\frac{M_j a}{r_e}-1\right)\right]\left(\frac{\alpha^2M_j^2}{r_e^2}\right)+\frac{\beta\alpha^2M_j^2}{r_e^2}\right]\exp\left(-\alpha\left(\frac{M_j a}{r_e}-1\right)\right)\right\} \quad \text{..... (5)}$$

At absolute zero, $T = 0$, $a = a_o$ the equilibrium lattice constant. At this value,

$$\left[dE(a)/da\right]_{a_o} = 0, \quad \text{..... (6)}$$

Also the bulk modulus B_0 within this imposed condition can be written as;

$$B_0 = \frac{a_o^2}{9Vc}\left[d^2E(a)/da^2\right]_{a_o} \quad \text{..... (7)}$$

The parameters of our pair potential function have been determined by using equations (3) to (7) and the lattice parameter, bulk modulus and the internal energy of the selected cubes for this `study. The values obtained for these parameters are presented in table one.

111. EXPRESSION FOR THE COEFFICIENTS OF THERMAL EXPANSION

Two atoms are bonded together by an atomic pseudo spring with proper potential energy. The atoms are stationary at absolute zero and they start to vibrate as temperature increases. At temperature T, the increasing energy ΔE of one dimensional diatomic motion is described as $\frac{1}{2}k_B T$, where k_B represents the Boltzmann`s constant. The diatom vibration with their repulse and attractive vibration amplitude r_1 and r_2, the average distance of this diatomic system changes from r_e to $\left[\frac{r_2 - r_1}{2}\right]$ when the temperature increases from T_1 to T_2. In comparison with experimental data, T_1 is set to be 0K. Therefore, the thermal expansion coefficient of the diatomic system is described as follows;

$$CTE = \frac{\left(\frac{r_2 - r_1}{2}\right) - r_e}{r_e\left(T_2 - T_1\right)} \quad \text{...} (8)$$

Since the energy change when the temperature changes, this energy change energy expressed in terms of Boltzmann constant is given as

$$\Delta E = E_2 - E_1 = \frac{1}{2}k_B T \quad \text{..} (9)$$

where E_1 and E_2, respectively represent the initial energy at T_1=0K, the energy at temperature T_2. In terms of the potential function, this is represented as

$$-\phi_e\left[1 + \beta\left(\frac{r_{ij}}{r_e} - 1\right)\right]e^{-\alpha\left(\frac{r_{ij}}{r_e} - 1\right)} + \phi_e = \frac{1}{2}k_B T \quad \text{.........................} (10)$$

By solving equation (10) the vibration amplitudes r_1 and r_2 are determined as

$$r_2 = \left[-\{\alpha - \beta\} + \sqrt{(\alpha - \beta)^2 + \left(\alpha\beta - \frac{\alpha^2}{2}\right)\left(\frac{k_B T}{2\phi_e}\right)} \Big/ 2\left(\alpha\beta - \frac{\alpha^2}{2}\right)\right] r_e + r_e \quad \text{............} (11)$$

$$r_1 = \left[-\{\alpha - \beta\} - \sqrt{(\alpha - \beta)^2 + \left(\alpha\beta - \frac{\alpha^2}{2}\right)\left(\frac{k_B T}{2\phi_e}\right)} \Big/ 2\left(\alpha\beta - \frac{\alpha^2}{2}\right)\right] r_e + r_e \quad \text{...........} (12)$$

The coefficient of thermal expansion can be deduced from r_2 and r_1 as

$$CTE = \sqrt{(\alpha - \beta)^2 + 4\left(\alpha\beta - \frac{\alpha^2}{2}\right)\left(\frac{k_B T}{2\phi_e}\right) \Big/ 4T^2\left(\alpha\beta - \frac{\alpha^2}{2}\right)^2} \quad \text{.........................} (13)$$

Equation (13) shows that the coefficient of thermal expansion of metals depends solely on the three potential parameters.

3.0 TEMPERATURE DEPENDENT PAIR POTENTIAL FUNCTIONS

There are two terms in this modulated pair potential function, one representing the attractive energy and the other representing the repulsive energy between atoms. In order to fully describe the thermal behavior of metals, a temperature related function should be included in the function. This is given as $A(T)$. In this study, the temperature related function is expressed as a second order polynomial, $A(T) = a_0 + a_1T + a_2T^2$, where a_0, a_1 and a_2 are constant.

The pair potential function is now given as

$$\phi_{(rij)} = -\phi_e\left[\left(a_0 + a_1T + a_2T^2\right) + \beta\left(\frac{r_{ij}}{r_e} - 1\right)\right]e^{-\alpha\left(\frac{r_{ij}}{r_e}-1\right)} \quad \ldots\ldots\ldots\ldots\ldots\ldots (14)$$

With increase in temperature from T_1 to T_2, corresponding energy increase is

$$\Delta E = E_2 - E_1 = -\phi_e\left[A(T) + \beta\left(\frac{r_{ij}}{r_e} - 1\right)\right]e^{-\alpha\left(\frac{r_{ij}}{r_e}-1\right)} + \phi_e A(T) = \frac{1}{2}k_BT \ldots\ldots\ldots\ldots\ldots (15)$$

By solving equation (15) the vibration amplitudes r_1 and r_2 are determined as

$$r_2 = \left[-\{\alpha A(T) - \beta\} + \sqrt{(\alpha A(T) - \beta)^2 + \left(\alpha\beta - \frac{\alpha^2 A(T)}{2}\right)\left(\frac{k_BT}{2\phi_e}\right)} \Big/ 2\left(\alpha\beta - \frac{\alpha^2 A(T)}{2}\right)\right]r_e + r_e \ldots\ldots\ldots (16)$$

$$r_1 = \left[-\{\alpha A(T) - \beta\} - \sqrt{(\alpha A(T) - \beta)^2 + \left(\alpha\beta - \frac{\alpha^2 A(T)}{2}\right)\left(\frac{k_BT}{2\phi_e}\right)} \Big/ 2\left(\alpha\beta - \frac{\alpha^2 A(T)}{2}\right)\right]r_e + r_e \ldots\ldots\ldots\ldots\ldots (17)$$

Hence the coefficient of thermal expansion can be written as.

$$CTE = \sqrt{(\alpha A(T) - \beta)^2 + 4\left(\alpha\beta - \frac{\alpha^2 A(T)}{2}\right)\left(\frac{k_BT}{2\phi_e}\right)} \Big/ 4T^2\left(\alpha\beta - \frac{\alpha^2 A(T)}{2}\right)^2 \quad \ldots\ldots\ldots (18)$$

·1V RESULTS

This section contains the experimental physical input, put together in table 1.0. The values of the EAM parameters put together in table 2.0.

Table1.0. Experimental physical input for the BCC metals.

Metals	Cohesive Energy ΔE (eV)	Lattice Constant a(A)	Vacancy Formation Energy E_{iv}^{F} (eV)	Elastic Constants $(in 10^{12} erg/cm^3)$			Bulk Modulus B $(in 10^{12} erg/cm^3)$
				C_{11}	C_{12}	C_{44}	
Li	1.630	3.4910	0.34	0.1480	0.1250	0.1080	0.1160
Na	1.1130	4.2250	0.42	0.0700	0.0610	0.0450	0.0680
K	0.9340	5.2250	0.39	0.0370	0.0314	0.0188	0.0320
Rb	0.8520	5.5850	0.28	0.0330	0.0286	0.0196	0.0310
Cs	0.8040	6.0450	2.28	0.0204	0.0198	0.0078	0.0200
V	5.3100	3.3000	2.20	2.2900	1.2100	0.4440	1.5700
Nb	7.5700	3.3000	2.60	2.4650	1.3450	0.2873	1.7020
Ta	8.1000	3.3000	2.80	2.6680	1.6110	0.8249	2.0000
Cr	4.1000	2.8800	1.91	3.5000	0.6780	1.0080	1.9010
Mo	6.8200	3.1500	3.00	4.6480	1.6160	1.0890	2.7250
·W	8.6600	3.1600	4.00	5.2270	2.0450	1.6060	3.2300
Fe	4.2900	2.8600	1.60	2.3310	1.3544	1.1783	1.6800

V DISCUSSION OF RESULTS

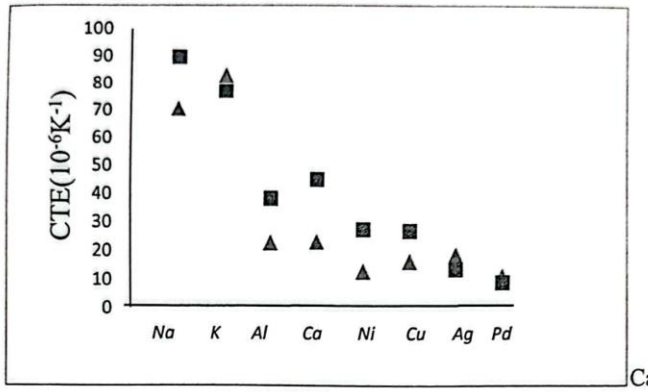
After substituting pair potential parameters of Table 4.1 into equation (7), the CTE of metals at room temperature (305K) are obtained and shown in Table 4.2. The calculated CTE shows reasonable agreement with the experimental value. Applying further equation (7) to calculate the CTE at different temperature, the results become insensitive to temperature and the prediction does not match experimental results anymore. Figure 4.1 shows the comparison of the temperature dependent thermal expansion of cubic metals. In reality, the CTE of metals is much smaller at a low temperature than that at room temperature, and the CTE becomes larger when the temperature is close to the melting point. This is due to the changes in bond strength and the shifting of the average position of atomic vibration. However, in the analytic solution using the original modulated first order polynomial pair potential function, the calculated CTE are in good agreement with experimental value and in case of some metals Na, Al and Ca there are little deviation from the experimental value. The temperature dependent using modified first order polynomial pair potential function is compared with modified Morse potential and shown in figure 4.2, 4.3, 4.4and4.5. Therefore, a modified modulated first order polynomial pair potential function with temperature-related parameters is a must in describing the thermal expansion behavior of metals. Using the derived expression for CTE from first order polynomial modulated pair potential at room temperature (305K), the calculated values of CTE were given table 4.2 after substituting the parameters in table 4.1 and were compared with the experimental values.

Table 4.1 Parameters for cubic metals applied in this study.

Metals	α	β	ϕ_a
Cu	10.2066	11.2580	1.0619
Ag	11.8322	12.5044	0.9382
Pd	12.8074	13.3194	1.2663
Pt	12.9148	13.4115	1.8825
Rh	12.0360	12.6912	1.0285
Ni	10.1590	11.2242	1.3559
K	10.2145	14.9505	0.1826
Na	9.12340	13.6797	0.2063
Ca	8.94920	10.4340	0.5338
Al	9.35986	10.6838	0.9879

In which the experimental value were obtained from Hong Mei Jin and Ping Wu (2002), Davis (1990), Gray (1973), Lide (2002), Metals Handbook 10th edition, I.V. Pirog and T.I. Nedoseikina (2002) .

Figure 4.1 the calculated coefficient of thermal expansion of metals with experimental validation



Calculated value ■

Experimental value ▲

Table 4.3 The parameters of modified first order polynomial potential function

Metals	a_0	$a_1(10^{-5})$	$a_2(10^{-7})$
Cu	1.1528	-40.000	-1.9523
Ag	1.0958	-26.400	-1.9720
Al	1.1438	-15.002	-3.0021
Pd	1.0401	-7.5008	-0.5600
Pt	1.0738	-33.501	-4.7000
Rh	1.0544	-14.300	-1.9140
Ca	1.2241	-64.514	-2.9520
Ni	1.1458	-44.633	-3.4166
K	1.4538	15.000	-15.090
Na	1.4934	10.000	-6.0050

Here the graphical representations of temperature dependent thermal expansion of some cubic metals in figure 4.2, 4.3, 4.4 and 4.5 are given below.

Figure 4.2 A graph of temperature dependent CTE for Calcium

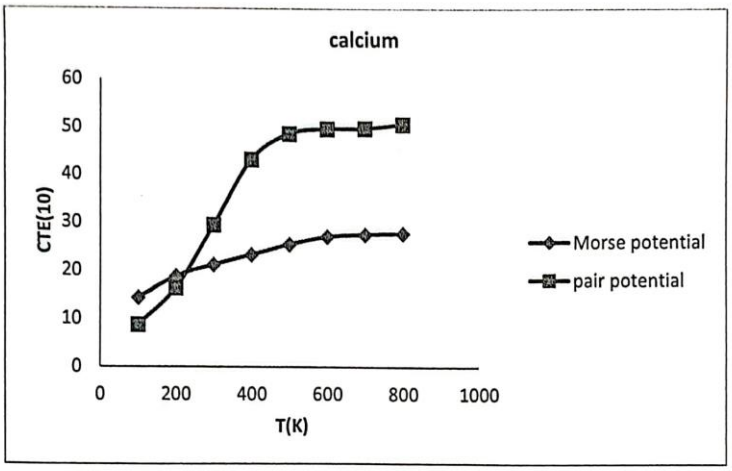


Figure 4.3 A graph of temperature dependent CTE for nickel

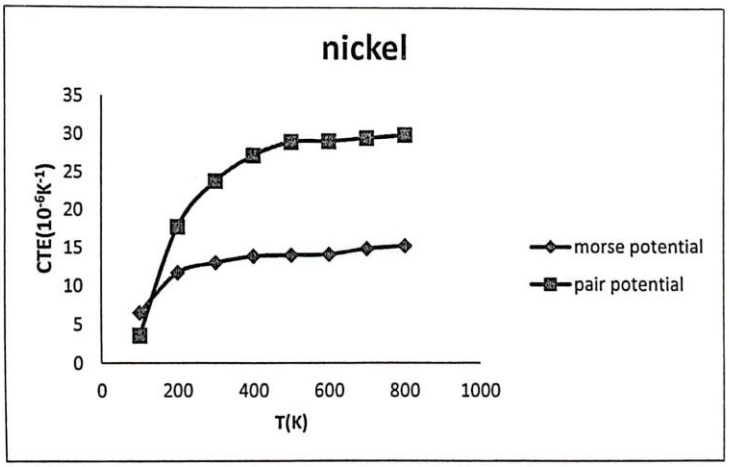
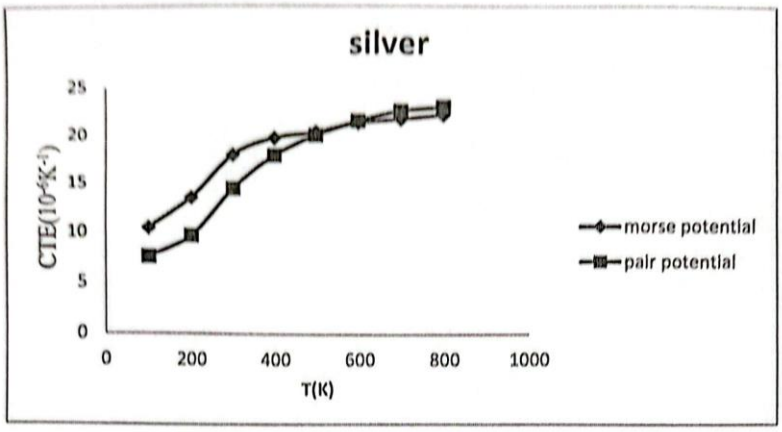


Figure 4.5 A graph of temperature dependent CTE for silver



4.1 Conclusion

The aim of this work was to propose a pair potential in form of anharmonic potential which when modified to contain a temperature dependent term can be to obtain the CTE for some selected metals (Cu, Ag, Pd, Pt, Rh, Ni, K, Na, Ca, Al). The result showed that this modulated first order pair potential can adequately be used for this purpose as the resulted generated cooperate finally with the experimental result used in Morse potential.

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