Advances in Physics Theories and Applications
ISSN 2224-719X (Paper) ISSN 2225-0638 (Online)
Vol 8, 2012

Solution of Morse Potential for Face Centre Cube Using Embedded Atom Method

Abajingin, D. D.
Department of Physics and Electronics, Adekunle Ajasin University. Akongba-Akoko. Ondo-State. Nigeria.
E-mail: abajingindd @yahoo.com

Abstract

The various methods as used in generating values for the Morse potential parameters involved heavy computational simulations and complex fitting to bulk properties of crystals. These identified problems had prompted us to evolve an analytical method for determining the Morse potential parameters for face centered cubic. In this method, the equilibrium values of the bulk parameters of some selected face centered cubic are fitted to the embedded atom method parameters. The experimental physical inputs are made up of the bulk modulus, lattice constants, elastic constants and the vacancy formation energy. Numerical calculations carried out to determine the fitness of the total energy from the Morse potential showed the fundamental properties of this potential. The values of the Morse potential parameters obtained from the derived analytic expressions were used to calculate the compressibility and the *Grüneisen's* constant for face centered cubic, (fcc), crystals at room temperature. The results generated for these parameters agreed well with the experimental values found in literature.

KEY WORDS: Morse Potential, Face Centered Cube, Embedded Atom Method, Lattice Constant, Elastic Constants, Vacancy Formation Energy, *Grüneisen's* constant Compressibility.

Sponsor
Financial assistance was given by Adekunle Educational Foundations.

Introduction

The Morse potential has it foundational principle on the anharmonic effects of the atoms within the lattice constant. The functional form of this potential is suppose to predict the energy values between two neighbouring atoms accurately well, when values of the associated parameters are accurately predicted. Available values of these parameters were often obtained from anharmonic effects contained in X-ray Absorption Fine Structure (XAFS) which influences the physical information taken from the spectra,[1, 2, 3]. Also Morse potential parameters have been determined by fitting the first and the second derivatives of the total energy of a metal into the compressibility, dislocation energy and elastic constants of the crystal at absolute pressure and temperature, [4, 5].

The heavy computational simulations demanded by these methods and the complex fitting to bulk properties of selected crystals, prompted us to by bypass these common methods and evolve a much simpler analytical method. In this method the total energy of crystal at ground state is obtained through discrete summation of the pair potential function, in this case, the Morse potential, over all the atoms in the crystal and, fitted to the ground state energy functions within the embedded atom method. This study is also designed to determine two crystal properties whose expressions depend effectively on Morse potential parameters. These EAM parameters are the lattice constants, elastic constants, bulk modulus, the vacancy formation energy, first and second derivatives of the potential energy functions, needed to specify the total energy of a crystal, [6].

The EAM is a technique widely used for constructing many-body potential models for metals. The required functions needed to completely specify the background theory of the EAM are analytically determined. This constitutes major reason in this study for fitting the desired Morse parameters to the EAM parameters.

Solution of Morse Potential for Face Centered Cube (fcc)

The pair potential energy $\phi(r_{ij})$ of two atoms i and j separated by a distance r_{ij} is given in terms of the Morse potential function as

$$\phi(r_{ij}) = D\left\{\exp(-2\alpha(r_{ij} - r_e)) - 2\exp(-\alpha(r_{ij} - r_e))\right\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

where α and D which are constants, respectively have the dimensions of reciprocal distance and energy. These are the two parameters whose values are to be determined analytically. The value of parameter r_e is fixed to be equal to the equilibrium distance between two atoms i and j within the first nearest neighbour concept, given as $r_e = a_o/\sqrt{2}$, a_o is the equilibrium lattice constant of the crystal.

The total energy $E(r)$ of a crystal whose atoms are at room temperature can be obtained by summing equation (1) over the entire atoms of the crystal. This is done by choosing one atom in the lattice as an origin, and calculating its interaction with other atoms in the crystal. The result obtained from such summation should be multiplied by N/2, where N is the atomic number of the metal, [7]. The functional form of the total energy $E(r)$ of a crystal in terms of the Morse potential, from this procedure is given as

$$E(r) = \frac{1}{2}ND\sum_{i,i\neq j}\left\{\exp(-2\alpha(r_{ij} - r_e)) - 2\exp(-\alpha(r_{ij} - r_e))\right\} \ldots\ldots\ldots\ldots (2)$$

In equation (2), atom i is taken as the origin or the reference atom over which the summation is performed.

Within the first nearest neighbor atoms concept, the summation in equation (2) reduces to

$$E(r) = \frac{1}{2}ND\left\{\exp(-2\alpha(r - r_e)) - 2\exp(-\alpha(r - r_e))\right\} \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Evaluating equation (3) at $r = r_e$, gives the equilibrium energy of the crystal, thus

$$\frac{1}{2}ND = -U_o \ldots\ldots\ldots\ldots\ldots\ldots (4) \quad \text{and} \quad D = \frac{-2U_o}{N} \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

where U_o is the equilibrium internal energy of crystal.

The total energy equation for any crystal within the EAM theory is given as the sum of the embedded energy required to embed an atom into the lattice and the summation of the pair potential energies between all the existing atoms in the crystal. This total energy representation is given as;

$$E(r) = F(\rho(r)) + \frac{1}{2}\sum_{i,(j\neq i)}\phi(r_{ij}) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

Within this framework, the EAM total energy equation can now be captioned as

$$\frac{1}{2}ND\left\{\exp(-2\alpha(r_{ij} - r_e)) - 2\exp(-\alpha(r_{ij} - r_e))\right\} = F(\rho(r)) + \frac{1}{2}\sum_{i,(i\neq j)}\phi(r_{ij}) \ldots\ldots\ldots (7)$$

The pair potential function is thus given as

$$\phi(r) = \left(ND\left\{\exp(-2\alpha(r - r_e)) - 2\exp(-\alpha(r - r_e))\right\} - 2F(\rho(r))\right)/12 \ldots\ldots\ldots (8)$$

The first and the second derivatives of equation (8) evaluated at $r = r_e$ and at $\rho = \rho_e$, are respectively

$$\phi'(r_e) = -\frac{1}{6}\left(F'(\rho_e)\rho'(r_e)\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (9)$$

$$\phi''(r_e) = \frac{1}{6}\left\{ND\alpha^2 - \left[F'(\rho_e)\rho''(r_e) + F''(\rho_e)\left(\rho'(r_e)\right)\right]^2\right\} \ldots\ldots\ldots\ldots\ldots (10)$$

The values for ϕ' and ϕ'' are fully determined if the values of the first and the second derivatives of the embedded energy function $F(\rho)$ are known, and those of the electron density function $\rho(r)$ are specified. The embedded energy function, [8] used, is given as

$$F(\rho) = F(\rho_e)\left(\frac{\rho(r)}{\rho_e}\right)^{\lambda_G} \exp\left(-\alpha_G\left(\frac{\rho(r)}{\rho_e}\right)\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

The first and the second derivatives of the embedded energy function are readily obtained from equation (11), while the first and the second derivatives of the electron density are obtained directly from the original EAM equations, [6]. The following are the expressions for these parameters, derivable from the EAM equations;

$$\rho'(r_e) = \frac{3V_{11}}{r_e} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (12)$$

$$\rho''(r_e) = \frac{6}{F'(\rho_e)}\left(\frac{3aB_e}{4} - \phi''(r_e) - \frac{3}{2r_e^2}\left(\Omega_e(C_{12} - C_{44})\right)\right) \ldots\ldots (13)$$

$$\phi(r_e) = \frac{\{E_c - F(\rho_e)\}}{6} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (14)$$

$$\phi'(r_e) = \frac{-F'(\rho_e)}{2r_e}\sqrt{\frac{\Omega_e(C_{12} - C_{44})}{F''(\rho_e)}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (15)$$

$$\phi''(r_e) = \frac{a}{8}\{3B_e - 2C_{11} + 4C_{12} + 4C_{44}\} + \frac{23F'(\rho_e)\rho(r_e)}{12r_e} \ldots\ldots (16)$$

where $\phi(r_e)$, $\phi'(r_e)$, and $\phi''(r_e)$ are respectively the expressions for the first and the second derivatives of the pair potential function evaluated at equilibrium inter atomic distance r_e. $F(\rho_e)$, $F'(\rho_e)$ and $F''(\rho_e)$ are respectively the first and the second derivatives of the embedded energy function evaluated at equilibrium electron density ρ_e. C_{11}, C_{12} and C_{44} are elastic constants of fcc metals, V_{11} is the embedded atom method parameter and Ω_e is the equilibrium volume per atom.

The expression for Morse potential constant α is now determined by comparing equations (9) and (17), the result of this comparison gives

$$\alpha = \sqrt{\left\{\frac{6a}{8ND}\left[3B_e - 2C_{11} + 4C_{12} + 4C_{44}\right] + \frac{23F'(\rho_e)\rho'(r_e)}{12NDr_e} + \frac{F''(\rho_e)[\rho'(r_e)]^2 + F'(\rho_e)\rho''(r_e)}{ND}\right\}} \ldots (17)$$

Application of Morse Potential

In this section, we apply the Morse potential parameters as obtained from equations (5) and (17) to calculate the compressibility and the $Grüneisen's$ constant. Several expressions have been proposed in literature to calculate these parameters, [8,9,10]. In this study, the expressions for the compressibility β and the $Grüneisen's$ constant γ as given in [8] are used. These are respectively given in equations (18) and (19).

$$\frac{9v}{\beta} = r_e^2 \left.\frac{d^2E(r)}{dr^2}\right|_{r=r_e} \ldots\ldots\ldots (18) \qquad \gamma = -\frac{r_e}{6}\left.\frac{d^3E(r)}{dr^3}\right|_{r=r_e} \left.\frac{d^2E(r)}{dr^2}\right|_{r=r_e}^{-1} \ldots\ldots\ldots (19)$$

These expressions depend solely on the three Morse potential parameters, D, r_e and α.

Experimental Physical Inputs

The experimental physical inputs, which consist; the lattice constants, a in the unit of ($\dot{A}$), the bulk modulus, B in the unit of ($10^{12} erg / cm^3$), and the cohesive energy, E_c in unit of (eV) are respectively taken from Kittel, [11] and Rose, et al., [12]. Other experimental physical inputs are the elastic constants, C_{11}, C_{12} and C_{44} in unit of ($10^{12} erg / cm^3$) and the vacancy formation energies, E_{iv}^F in unit of (eV). The values to these parameters are taken from Smith et al., [13]. The values for these inputs are put together in table one.

Calculated EAM Parameters

These are the values for the first and second derivatives of the pair potential functions, the values of the first and second derivatives of the electron density obtained from the EAM equations, (12-16). The values are put together in table two. Table three contains calculated values of the embedded energy function parameters. These tables are shown in appendix one.

Results

The results generated from this study are presented in tables 4, 5 and 6. Table 4 contains the values of the two parameters, (α and D.) in the Morse potential. Tables 4 and 5 respectively contain the calculated values of the *Grüneisen* constant and the compressibility constant for the selected fcc metals. All these are put together in appendix two. The functional fit of the total energy equation from the Morse potential are shown in figures 1 and 2 for the seven selected fcc metals. These figures are shown in appendix three.

Discussion of Results

Morse potential as shown in equation one is adopted here to describe the relationship between the potential energy and the atomic distance of a diatomic system. The theoretical background for this study lies fully in fitting the ground state of the total energy of the crystal coined from Morse potential to the ground state of the total equations of the EAM as shown in equation (6).

The values of the Morse potential parameters computed from this theoretical frame work for the seven selected fcc metals compared favourably with values from other theoretical studies,[15 ,16]., respectively marked (*) and (**) in table 4. The values of α from this study differ slightly by 1% from those from reference [15] and differ by 0.05% from those of reference [16]. The values of D differ respectively from those of reference [15] and reference [15] by 1% and 0.1%.

The functional fits for the total energy obtained from the Morse potential, and shown in figures 1 and 2, show the fundamental properties of this potential. The cohesive energy for each of the selected fcc metal are adequately predicted

The values of the *Grüneisen* constants are put together in table 5. Column two contains the values of this constant from this study as calculated from equation (20), while the experimental data, [17], are contained in column three. Values of this constant from available theoretical studies, [18 and 19] are respectively shown in columns four and five. The predicted values of *Grüneisen* constant from this study are in good agreement with experimental data and those from the theoretical studies. [19]. This table shows that these values have been successfully reproduced for Ni, Cu and Pd. The predicted values of the *Grüneisen* constants are slightly lower than those from both the referenced theoretical and experimental values for Pt, Au and Ag but give a good agreement with the experimental value for Al. taken from Marini [20].

Table 6 contains the values of the compressibility constants. The values in column two are those from this study and calculated from equation (19). The values are in good agreement with the experimental, [13].

Conclusion

The results reported in this study are satisfactory in view of the simple machinery of calculations required when one uses the analytic functions of the EAM. This approach relates the anharmonic effect which is the foundational concept of the Morse potential to simple pair potential function which exists naturally between paired atoms. The correct predicted experimental values of the cohesive energy for alkali metals within the framework of this study furnishes us with a path of obtaining the parameters of analytic pair potential functions from other models.

REFERENCES

1. Miyannga, T. and Fujikawa, T. Quantum statistical Approach to Debye – Waller factor in EAXFS, EELS and ARXPS 11: Application to one dimensional model. Journal of Physics Society. Japan. Vol. 63 1036 and 3683. (1994).
2. Nguyen, V. A., Nguyen, C. T., Nguyen, B. J., and Ngo, N. G. Calculation of Morse Potential for Diamond Crystals. Application to Anharmonic Effective Potential, VNU Journal of Science, Mathematics-Physics. Vol. 24 Pg. 125-131. (2008).
3. Hung, N.V., and Duc, N. B., and Frahm, R. A New Anharmonic factor and XAFS including Anharmonic Contributors. Journal of Physics Society. Japan. Vol. 72, 1254. (2003)
4. Pirog, I. V., Nedoseikina, T.I., Zarubin, I.A and Shuvaev, A. T. Anharmonic pair potential study in face centered structure metals**,** Journal Physics Condense Matter, Vol. 14, 1825. (2002).
5. Nedoseikina, T. I, and Pirog, I.V. Study of effective pair potentials in cubic metals. Physica. B, Condensed matter, Vol: 334, Pages: 123-129. (2003).
6. Daw, M. S., Baskes, M. I. Embedded Atom Method: Derivation and application to Impurities, Surface, and other Defects in Metals. Journal of Physical Review. B. Vol. 29, No 12, Pg 6443-6453. (1984).
7. Nguyen, V. H, A method for calculation of Morse Potential for FCC, BCC, HCP Crystals: Applied to Debye-Waller Factor and Equation of State. Communication in Physics, vol. 14 No 1 Pg -14. (2004).
8. Idiodi, J. O. A and Obodi, G. N. The Separable Potential Method and its Connection with the Embedded-Atom Method. Phys. Stat. Sol. (b) 177, 281. (1993).
9. Kachhava, C. M and Sexana, S. C. Thermal Expansion and Gruneisen constant of Crystals: Indian Natural Science Academy. 43, 110. Phys., Vol. 40, Pg 273. (1963).
10. Godwal, B. K, Sikka, S. K and Chidambaram, R. (1983). *Phys. Rep.***102** 121
11. Grover R, Keeler R N, Rogers F J and Kennedy G C J.Phys. *Chem. Solids* **30** 2091. (1969).
12. Kittel, C. Introduction to Solid State Physics, John Wiley and Son, 8th Edition New York. (2005).
13. Rose, H., Smith, J. R., Guinea, F., and Ferrante, J. Universal Features of the equation of State. Journal of Physical Review. B. Vol.29. 2963. (1984).
14. Smith, J. R., Perry, T., Banerjea, A., Ferrante, J., and Bozzolo, S. I. Equivalent-crystal theory of metal and semiconductor surfaces and defects. Journal of Physical. Review. B. vol.44. 6444. (1991).
15. Girifalco, L. A, and Weizer, V. A., Application of Morse Potential Function to Cubic Metals. Journal of Physical. Review. Vol. 114 No 3. (1959)
16. Kachava, C.M and Sharma, K.S. Application of Morse Potential to Molecular-Metallic-Frame Work; Indian Journal of Physics. Vol. 45. A, No 5, Pg 425-431. (1979).
17. Gschneidner, K. A. *Solid state phys. advances in research and applications,* edited by F Seitz and D Turnball (New York: Academic Press) **16** p. 412. (1964).
18. Pandya, C. V., Vyas, P. R., Pandya, T.C. and Gohel, V. Volume variation of. *Grüneisen* Parameters of fcc transition metals. Bull. Material Science. Vol. 25, No1. pp 63-67. (2002).
19. Barrera, G.D., and Batana, A. Lattice Dynamics, Thermal expansion, and third order elastic constants of semi-noble metals. Journal of Physical. Review. B47, 8588. (1993).

20. Marini A. The Gruneisen parameter for aluminum in the temperature ranges 0.3-1.1 K. *PACS numbers: 74.25.-q, 65.40.-b.* (2008).

Appendix 1.

Tables of Experimental Physical Inputs

Table 1: Experimental physical inputs for the seven selected fcc metals

Elements	Cohesive Energy E_c (eV)	Lattice Constants $a(\dot{A})$	Vacancy Formation Energy E^F_{1v} (eV)	Elastic Constants $(10^{12} erg/cm^3)$			Bulk Modulus B $(10^{12} erg/cm^3)$
				C_{11}	C_{12}	C_{44}	
Ni	4.44b	3.510b	1.60c	2.612c	1.508c	1.317c	1.876
Cu	3.50b	3.615b	1.30c	1.762c	1.249c	0.818c	1.420
Pd	3.94b	3.890b	1.40c	2.341c	1.761c	0.712c	1.955
Pt	5.85b	3.920b	1.30c	3.580c	2.536c	0.774c	2.884
Au	3.78b	4.070b	0.96c	2.016c	1.697c	0.454c	1.803
Ag	2.96b	4.080b	1.19c	1.314c	0.973c	0.511c	1.087
Al	3.34b	4.040b	0.66c	1.143c	0.619c	0.316c	0.794

Table 2: Calculated values of the embedded atom method parameters

Metals	$\phi(r_e)$	$\phi^{/}(r_e)$	$\phi^{//}(r_e)$	$\rho^{/}(r_e)$	$\rho^{//}(r_e)$	V_{11}
Ni	0.7061	0.8246	0.8795	0.8637	-1.9786	0.7145
Cu	0.6223	1.2652	-0.9335	1.5325	-3.1551	1.3039
Pd	0.0050	0.5209	2.0356	2.3338	1.7290	2.1398
Pt	0.6263	1.7338	0.1271	2.1338	-2.3775	1.9715
Au	0.1200	0.6404	1.6116	2.4368	2.0725	2.3377
Ag	0.5462	1.4169	-1.3468	1.9295	-3.4596	1.8555
Al	0.5279	0.7178	-0.5498	1.1584	-2.3858	1.1031

Table 3: Calculated values of the embedded energy function parameters

Metals	α_G	λ_G	$F(\rho_e)$	$F^{/}(\rho_e)$	$F^{//}(\rho_e)$
Ni	0.0666	0.7268	-8.6767	-5.7284	2.5244
Cu	0.0414	0.7262	-7.2335	-4.9535	1.8608
Pd	0.3065	0.6438	-3.9700	-1.3391	2.1042
Pt	0.1935	0.7009	-9.6080	-4.8751	4.2606
Au	0.3041	0.6545	-4.5002	-1.5769	2.3928
Ag	0.0206	0.7270	-6.2373	-4.4060	1.4221
Al	0.1488	0.7201	-6.5077	-3.7178	2.5622

Appendix 2.

Table 4: Calculated values of Morse potential parameter.

Metals	Ni	Cu	Pd	Pt	Au	Ag	Al
α	1.4432 1.4199^* -	1.4342 1.3123^* 1.3588^{**}	1.6464 - -	1.6474 - -	1.6511 1.5830^* -	1.4506 1.1836^* -	1.1613 1.0341^* 1.1646^{**}
D	0.3171 0.4205^* -	0.2414 0.3429^* 0.3364^{**}	0.1713 - -	0.1500 - -	0.0957 - -	0.1260 0.3323^* -	0.5138 0.2703^* -

Table 5: Values of *Grüneisen* constants γ for the selected fcc metals.

Elements	Authors' Values	Experimental Values	Other Theoretical Values for γ	
			Barrera and Batana	Pandya et al
Ni	1.7909	1.830	1.620	2.770
Cu	1.8305	1.970	1.840	1.930
Pd	2.2643	2.280	2.180	2.180
Pt	2.2832	2.560	2.500	2.640
Au	2.3759	3.060	2.770	1.190
Ag	2.0924	2.360	2.220	3.280
Al	1.6588	1.700^{***}	-	-

Table 6: Values of Compressibility for the selected fcc metals

Elements	Ni	Cu	Pd	Pt	Au	Ag	Al
Present Values	0.5473	0.7231	0.5252	0.3560	0.5695	0.9446	1.2932
Experimental Values	0.5380	0.7300	0.5530	0.3590	0.5770	0.9930	0.9930

Appendix 3.

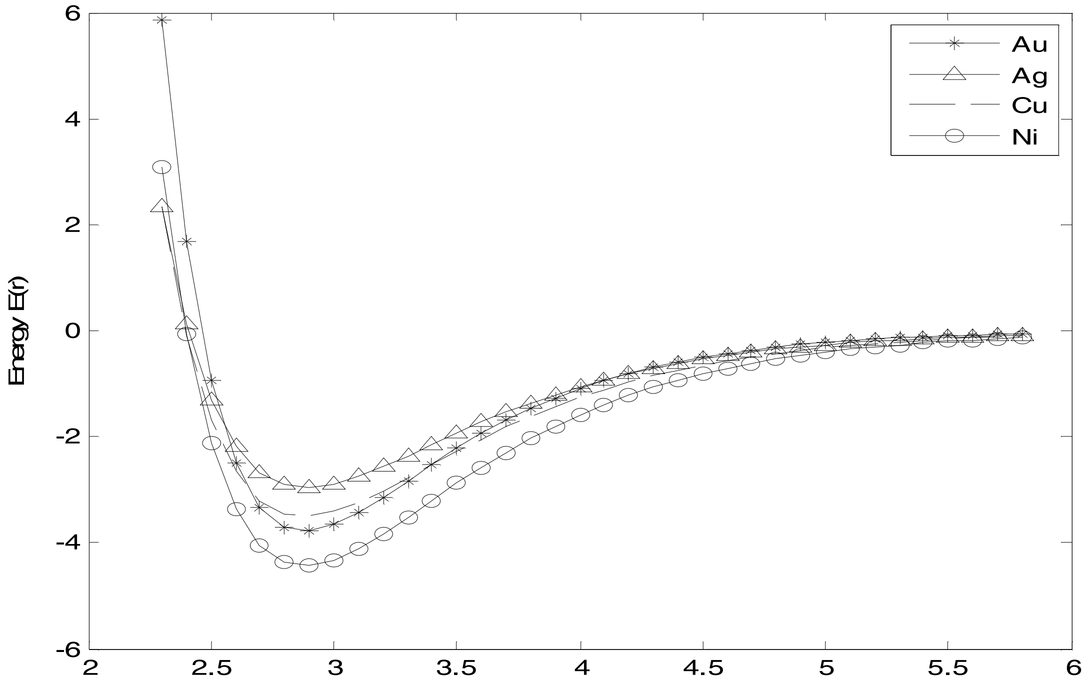

Fig.1 Graph of Toyal Energy Total Energy E(r) against Interatomic Distance r for Au, Ag, Cu and Ni

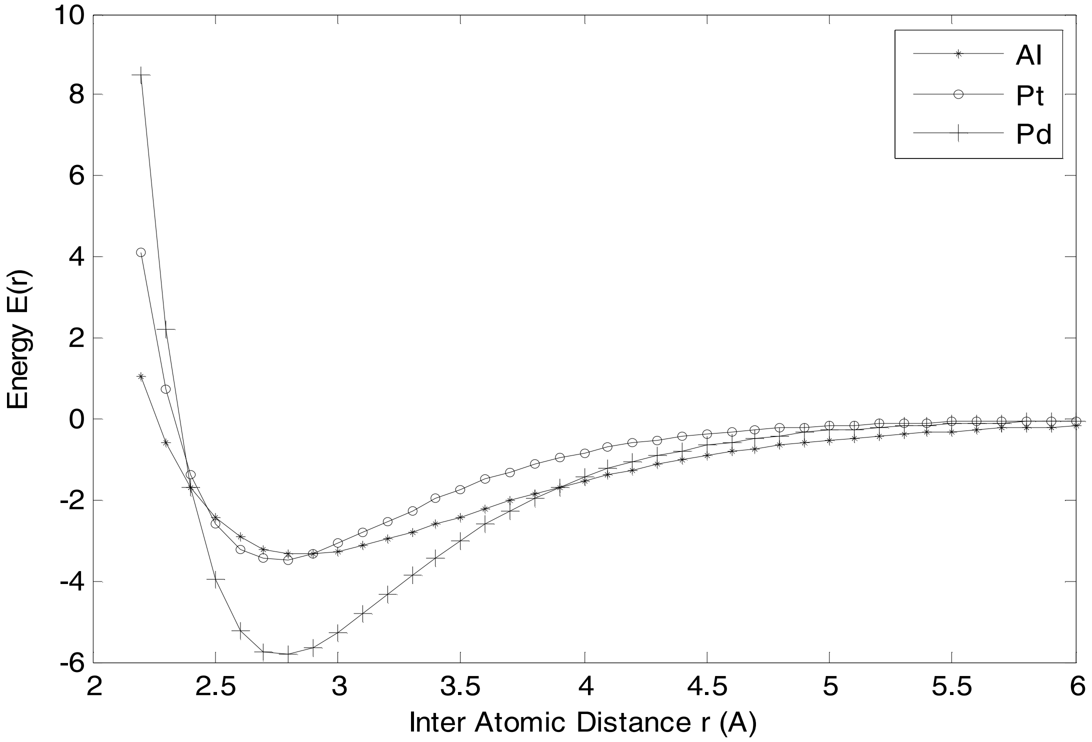

Fig.2. Graph of Total Energy against Inter-Atomic Distance r
for Al, Pt and Pd

This academic article was published by The International Institute for Science, Technology and Education (IISTE). The IISTE is a pioneer in the Open Access Publishing service based in the U.S. and Europe. The aim of the institute is Accelerating Global Knowledge Sharing.

More information about the publisher can be found in the IISTE's homepage:
http://www.iiste.org

The IISTE is currently hosting more than 30 peer-reviewed academic journals and collaborating with academic institutions around the world. **Prospective authors of IISTE journals can find the submission instruction on the following page:** http://www.iiste.org/Journals/

The IISTE editorial team promises to the review and publish all the qualified submissions in a fast manner. All the journals articles are available online to the readers all over the world without financial, legal, or technical barriers other than those inseparable from gaining access to the internet itself. Printed version of the journals is also available upon request of readers and authors.

IISTE Knowledge Sharing Partners

EBSCO, Index Copernicus, Ulrich's Periodicals Directory, JournalTOCS, PKP Open Archives Harvester, Bielefeld Academic Search Engine, Elektronische Zeitschriftenbibliothek EZB, Open J-Gate, OCLC WorldCat, Universe Digtial Library , NewJour, Google Scholar