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Analytic functions for calculating binary alloys of FCC metals

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Abstract

The problem studied in this paper is that of obtaining appropriate electron density function and a pair potential function for an FCC metal within the EAM format. The approach adopted is to use the experimental dilute limit heats of solution of the binary alloys of FCC metals as input parameters into Johnson analytical model, (*Phys. Rev. B. Vol. 39 12554 (1989) [1]*), for calculating the dilute limit heats of solution; and to try to determine the needed functions consistently. The functions that emerge from this approach satisfy the experimental information used as input and Johnson's equation for this same quantity, but they do not support the assumption, often employed in literature, of a single exponentially decreasing function of r for these functions. This then constitutes our explanation for the hitherto observed discrepancy between theory and experiment. **[See references 1 and 3].**

1.0 Introduction

The sole aim of this study is to obtain appropriate expressions for electron density and the pair potential functions which will best fit into the analytic nearest neighbour model within the embedded atom method (EAM). Before now the problem of obtaining such functions plague most of the research works focused on surface defects, alloy energetics and all allied defects. Johnson [1] in an attempt to solve this problem and advanced the inflexible single exponentially decreasing expressions for these two functions. The theoretical predictions for the dilute limit heats of solution to the binary alloys of the six selected FCC (Cu, Ag, Au, Ni, Pd and Pt) elements from the combination of the functions in the short range model of the EAM format showed a remarkable disagreement from the experimental values for this some alloy energetics [2, 3], that is, the wrong trends was predicted for the properties of the dilute-limit heats of solution of alloys involving Pd. This disagreement between theory and experiment persisted, particularly for the case of Pd in Ni, even in the recent analytic embedding atom potential model including a long range force within the EAM format developed by Cai and Ye [3], which was carried out in the same spirit as Johnson's work. The failure of these two theoretical efforts has prompted us to re-examine the assumptions of a single exponentially decreasing function of r, often employed for the atomic density, in applications of the EAM. Hence developing a semi-empirical method, which can solve this problem within the analytic nearest neighbour within the EAM format, is put in place.

This work is arranged as follows: in section 2, appropriate EAM theory and EAM equations are briefly reviewed. The method of obtaining the expressions for the electron density and the pair potential functions is given in section 3. Calculated values of the parameters as surfaced in each of the functions are tabulated and presented in section *iv*, and concluding remarks are made in section 5

2.0 EAM theory

Daw and Baskes [4] originally evolved the EAM theory, and its basic ideals can be interpreted in the framework of density-functional theory as developed by Hohenberg and Kohn [5]. The significant contribution of Baskes et al, is that they have used the ideals within the density functional theory to write out the total internal energy for the collection of atoms constituting the metallic solid, the embedding energy plus a core-core repulsive potential that can be fully determined by experimental data. From this, the basic equations of EAM [4] as expressed by Foiles et al]6] for a monatomic metallic solid are given as

$$E_{tot} = \sum_i F_i\left(\rho_{i,j}(r)\right) + \frac{1}{2}\sum_{i,j(j\neq i)} \phi(r_{i,j}) \tag{2.1}$$

$$\rho_{(h,i)} = \sum N_n \rho_h(r_{h,i}) \tag{2.2}$$

where E_{tot} is the total internal energy for the collection of atoms constituting the metallic solid.

$\rho_{(h,i)}$ is the electron density at the site of atom *i* due to the contribution from all the other atoms. The summation over *n* in equation (2.2) picks up the number of the neighbour atoms at some distance $r_{(h,i)}$ from atom *i*, each of these neighbour atoms contributing same density $\rho_h(r_{n,j})$ to the atom at position *i*.

$F_i(\rho)$ is the embedding energy as a function of density $\rho(r)$

$\phi(r_{i,j})$ is a two-body potential between atoms *i* and *j* separated by distance $r_{i,j}$.

Equation (2.1) as a function of *r* can be written as

$$E(r) = 6\phi(r) + F(\rho(r)) \tag{2.3}$$

Since there are twelve nearest neighbour atoms in unit cell, thus the ground state equation representing equation (2.3) is given as

$$E_c = F(\rho_e) + 6\phi_e \tag{2.4}$$

Thus

$$\phi_e = \frac{E_c - F(\rho_e)}{6} \tag{2.4b}$$

The first derivative of equation (2.3) with respect to *r* is $E'(r) = 6\phi'(r) + F(\rho)\rho'(r)$ (2.5)

and at $r = r_e$ this equation reduces to $0 = 6\phi'(r_e) + F(\rho_e)\rho'(r_e)$ (2.6)

The other EAM equations as related to the lattice constants expressed within the equilibrium conditions are

$$\frac{3}{4}aB_e = \phi''(r_e) + \frac{1}{6}F''(\rho_e)\left[\rho'(r_e)\right]^2 + \frac{1}{6}F'(\rho_e)\rho''(r_e) \tag{2.7}$$

Alternatively equation (2.7) can be written as

$$\frac{3}{4}aB_e = \phi''(r_e) + \frac{a}{4\Omega}F'(\rho_e)\left[2W_{11} - 8W_{12} - 5V_{11}\right] - \frac{a}{4\Omega}F''(\rho_e) \tag{2.8}$$

$$\frac{a}{4}C_{11} = \left[\frac{\phi'_e}{2r} + \frac{\phi''_e}{2}\right] + \frac{a}{4\Omega_e}F'W_{11} + t_1\frac{a}{4\Omega_e}F''V_{11}^2 \tag{2.9}$$

$$\frac{a}{4}C_{12} = \left[\frac{-5\phi'_e}{4r} + \frac{\phi''_e}{4}\right] + \frac{a}{4\Omega_e}F'W_{12} + t_2\frac{a}{4\Omega_e}F''V_{11}^2 \tag{2.10}$$

$$\frac{a}{4}C_{44} = \left[\frac{-5\phi_e'}{4r} + \frac{\phi_e''}{4}\right] + \frac{a}{4\Omega_e}F'W_{12} + t_3\frac{a}{4\Omega_e}F''V_{11}^2 \qquad (2.11)$$

B_e and C_{11}, C_{12} and C_{44} are respectively the bulk and the elastic constant written in the Voigt notation. $r_e = a/\sqrt{2}$, and $\Omega_o = a^3/4$, are respectively the equilibrium nearest neighbour-distance, and the volume per atom in FCC lattice that has one atom per lattice and a is the equilibrium lattice constant. ϕ_e is a nearest neighbour repulsive pair potential whose first and second derivatives with respect to the radial distance r, are respectively ϕ_e' and ϕ_e'' {all quantities being evaluated at $r = r_e$}. $F'(\rho_e)$ and $F''(\rho_e)$ are the first and the second derivatives of the embedding function $F(\rho)$ with respect to the density evaluated at the equilibrium density ρ_e, V_{11}, W_{11} and W_{12}, are basic parameters of the EAM. Finally, E_{IV}^F is the mono vacancy formation energy. In the original EAM equations $t_1 = t_2 = 0$ and $t_3 = 0$. These equations are obtained at the equilibrium condition $r = r_e$. Equations (2.3) – (2.11) are sufficient to determine the known parameters ϕ_e', ϕ_e'', V_{11}, W_{11}, W_e, ρ_e' *and* ρ_e''. The expressions for these parameters are written below.

2.1 Expression for V_{11}

Since $t_1 = t_2 = \phi$ and $t_3 = 0$, subtract equation (2.11) from (2.10) we have that

$$\frac{q}{4}[C_{12} - C_{44}] = \frac{a}{\Omega}F''V_{11}^2 \qquad (2.12)$$

Thus
$$V_{11} = \sqrt{\frac{\Omega_o(C_{12} - C_{44})}{F''(\rho_e)}} \qquad (2.13)$$

2.2. Expression $\rho'(r_e)$ first derivative of electron density function

Daws and Baskes [4] had shown that $\rho'(\mathrm{r_e}) = \frac{3}{r_e}V_{11}$ (2.14)

Re arranging equation (2.14) in terms of V_{11} and substitute this in equation (2.13), we have that

$$\rho'(\mathrm{r_e}) = \frac{3}{r_e}\sqrt{\frac{\Omega_o(C_{12} - C_{44})}{F''(\rho_e)}} \qquad (2.15)$$

Re arrange equation (7), by making $\rho''(r_e)$ subject of formula then

$$\rho''(r_e) = \frac{6}{F'(\rho_e)}\left\{\frac{3aB_e}{4} - \phi''(r_e) - \frac{3F''(\rho_e)V_{11}^2}{2r_e^2}\right\} \qquad (2.16)$$

$\rho''(r_e)$ can absolutely be determined when $\phi''(r_e)$ is known.

2.3 Expression for $\phi'(r_e)$ and $\phi''(r_e)$ from the EAM Equations

From equation (2.6) we have that $\phi'(r) = \frac{F(\rho)\rho'(r)}{6}$ (2.17)

$$\phi_C' = \frac{-F'(\rho_e)V_{11}}{2r_e} \qquad (2.18)$$

where $\rho'(r) = \frac{3V_{11}}{r_e}$. Multiply equation (2.9) by 2 and equation (2.10) by 8, to respectively

obtain

$$\frac{2aC_{11}}{4} = \frac{\phi'_e}{r_e} + \phi'' + \frac{a}{4\Omega_e} F'(\rho_e) 2W_{11} + \frac{2a}{4\Omega_e} F'' V_{11}^2 \qquad (2.19)$$

$$\frac{8aC_{12}}{4} = \frac{-10\phi'_e}{r_e} + 2\phi'' + \frac{a}{4\Omega_e} F'(\rho_e) 8W_{11} + \frac{8a}{4\Omega_e} F'' V_{11}^2 \qquad (2.20)$$

Subtract equation (2.20) from equation (2.19), thereafter subtract the result from equation (2.8) to have

$$\frac{a}{4}\left[3B_e - 2C_{11} + 4C_{12} + 4C_{44}\right] = 2\phi''(r_e) - \frac{11\phi'(r_e)}{r_e} - \frac{5F'V_{11}}{a^2} \qquad (2.21)$$

Substitute equation (2.21) and the expression for $\rho'(r_e)$ in equation (2.16) to have

$$\phi''(r_e) = \frac{a}{8}\left[3B_e - 2C_{11} + 4C_{12} + 4C_{44}\right] - \frac{11F'(\rho_e)V_{11}}{2r_e^2} + \frac{5F'V_{11}}{a^2} \qquad (2.22)$$

Solving completely equation (2.22) becomes

$$\phi''(r_e) = \frac{a}{8}\left[3B_e - 2C_{11} + 4C_{12} + 4C_{44}\right] - \frac{3F'(\rho_e)V_{11}}{2r_e^2} \qquad (2.23)$$

From the equations above the bulk values of the parameters reflected in the EAM equations could be determined, the first and the second derivatives of the electron density and the pair potential functions can respectively be determined from equations (2.14 and 2.16) and (2.18 and 2.23).

3.0 Methods for obtaining the alloy functions

From the equations (2.1) and (2.2) put together above, three fundamental equations are clearly seen, these are (*i*) embedding energy function, $F(\rho)$, (*ii*) electron density function, $\rho(r)$ and (*iii*) pair potential function, $\phi(r)$.

Idiodi [7] have put in place these two forms of embedding function $F(\rho)$ for a monatomic FCC metal;

$$F(\rho) = F(\rho_e)\left\{\frac{\rho}{\rho_e}\right\}^{\lambda_0} \exp\left(-\alpha_e\left(\frac{\rho}{\rho_e} - 1\right)\right) \qquad (3.1)$$

$$F(\rho) = -f\left(\exp(\alpha_f - \exp\left(-\alpha_f\left(\frac{\rho}{\rho_e} - 1\right)\right)\right)^{\lambda_f} \qquad (3.2)$$

of the two functions we have adopted the embedding function of the form in equation (3.1) because it readily satisfies Foile's [6] characterization for embedding function. When we consider equation (2.3), the pair potential function takes the form

$$\phi(r) = \frac{E(r) - F(\rho(r))}{6} \qquad (3.3)$$

This clearly shows that the potential function is a function of r and ρ. The function $E(r)$ can easily be determined from Rose et al [10] energy equation. One basic deduction from equation (3.3) above is that for a specified value of the pair potential function there is always a compatible value of the electron density function. To be able to specify both the electron density and the pair potential functions, this concept of the compatibility of the values of this function is strongly stressed in this paper. In determining these compatible values for these parameters we have used the impurity expressions in the set of equations in Johnson's paper [1], with the provision that the value of the electron density function is not known but needs to be determined. The values of the electron density function thus obtained from the procedure are put together in table 4. These values are first substituted in equation (3.1) to obtain the corresponding values of the embedding function $F(\rho)$. The values obtained are thereafter substituted in

equation (3.3) to be able to determine the values for the pair potential function, which are put together in table 5.

The electron density curve fit show humps which can be said to be features of a Gaussian function while that of the pair potential is best matched by a polynomial as represented by (Poly. Series) line which is better than the exponential function as represented by (Expo. Series 1). These were accessed from a mat – lab programmer. From these observations we are representing the electron density function by a Gaussian function modulated by a polynomial of order seven while the pair potential function is represented by a polynomial of order seven, given as,

$$\rho(r) = \rho_e \left[1 + P_1\left(\frac{r}{r_e} - 1\right) + P_2\left(\frac{r}{r_e} - 1\right)^2 + P_3\left(\frac{r}{r_e} - 1\right)^3 + \ldots + P_7\left(\frac{r}{r_e} - 1\right)^7 \right] \exp\left(-\beta\left(\frac{r}{r_e} - 1\right)^2 \right) \tag{3.4}$$

$$\phi(r) = \rho_e \left[1 + h_1\left(\frac{r}{r_e} - 1\right) + h_2\left(\frac{r}{r_e} - 1\right)^2 + h_3\left(\frac{r}{r_e} - 1\right)^3 + \ldots + h_7\left(\frac{r}{r_e} - 1\right)^7 \right] \tag{3.5}$$

The choice of polynomial of order seven is most appropriate for this study, six metals are selected. So when an impurity metal is chosen there are five order metals which will in turn serve as the host metal, knowing fully that P_1 and h_1, P_2 and h_2 are respectively first and derivatives obtainable from EAM equations. The values of the parameters in the functions above are completely defined when the value of β have been determined. The formula derived for the determination of this parameter is given in appendix 1.

Five sets of simultaneous equations are to be solved in each case as the host metal varies from metal to metal respectively with a specified impurity metal. The values for the parameters in equations (3.4) and (3.5) are put together in tables 4 and 5 respectively.

4.0 Results and discussion

This model for the FCC metals requires some physical input parameters. These input parameters are the experimental values of the pure metal properties. They are used as input to determine the functions to be used for this work. These input parameters are the three bulk elastic constants (C_{11}, C_{12}, C_{44}), the bulk cohesive energy E_c, Lattice constants a_e, the Bulk modulus B_e, and the vacancy formation energy E_{iv}^F. The pure metal inputs used to determine the EAM functions are elastic constants (C_{11}, C_{12}, C_{44}) are in 10^{12} erg/cm^3. Bulk modulus in 10^{12} erg/cm^3 and the cohesive energies are in eV Elastic constants are in 10^{12} erg/cm^3. The vacancy formation energy E_{iv}^F is expressed in eV. The values for these parameters are taken from Ref. [1]. All these are put together in table 1.

Table 1: The physical input parameters

Metal	**Cohesive Energy (*eV*)**	**Lattice Constants** $a_e^0(A)$	**Vacancy Formation Energy** E_{iv}^F **(*eV*)**	**Elastic Constants**			**Bulk Modulus** B_e
				C_{11}	C_{12}	C_{44}	
Cu	3.54	3.615	1.30	1.700	1.225	0.758	1.380
Ag	2.85	4.090	1.13	1.240	0.934	0.461	1.040
Au	3.93	4.080	0.90	1.860	1.570	0.420	1.670
Ni	4.45	3.520	1.60	2.465	1.473	1.247	1.804
Pd	3.91	3.890	1.40	2.341	1.760	0.712	1.950
Pt	5.77	3.910	1.50	3.470	2.510	0.765	2.830

Table 2: Calculated EAM parameters for the bulk solid

$f_1,(eV),\alpha_f,\lambda_f$ are model parameters, $F(\rho_e)$ is the equilibrium value of the embedding function at ρ_e, while $F'(\rho_e)$ and $F''(\rho_e)$ are respectively the first and the second derivatives of the embedding function in equation (3.2). They are expressed in (eV), V_{11} (ρ_e) is the charge per unit length and determined from the bulk EAM equations. Idiodi [9] have given the method of obtaining the EAM parameters in table 2.

	Cu	***Ag***	***Au***	***Ni***	***Pd***	***Pt***
X	10.615	1.0635	1.0321	1.0594	1.0309	1.0459
$f_1(eV)$	122.6297	204.2813	3.2195	93.3626	2.2118	21.0187
a_f	0.1195	0.05800	1.30228	0.19054	1.37668	0.68213
λ_f	0.7273	0.7273	0.7273	0.7273	0.7273	0.7273
$V_{11}(\rho_e)$	-1.3472	-1.8948	2.2274	-0.7816	2.1971	2.0279
$F(\rho_e)(eV)$	-73626	-6.1666	-4.8382	-8.7051	-3.9234	-9.0136
$F'(\rho_e)[eV/\rho_e]$	-5.0411	-4.3560	-1.7011	-5.7470	-1.3263	-4.5718
$F''(\rho_e)[eV/\rho_e]$	1.8967	1.4065	2.4564	2.5178	1.9941	3.9881

Table 3: Calculated EAM Parameters for the Bulk Solids from this model.

ρ_e,ρ_e' and ρ_e'' are the equilibrium values respectively, for the electron density, its first and second derivatives with respect to *r*, at an atom site in a perfect crystal. The dimensions of ρ_e cancel (that is, it is a scaling factor). ϕ_e,ϕ_e' and ϕ_e'' are the values respectively, for the pair potential, its first and the second derivatives with respect to *r* and evaluated at the equilibrium value of the nearest – neighbour distance r_e. These values were determined using equations ((2.4b, 2.17 or2. 18 and 2.23), respectively.

	Cu	***Ag***	***Au***	***Ni***	***Pd***	***Pt***
$F(\rho_e)[eV]$	-7.3643	-6.1665	-4.8356	-8.7025	-3.9234	-9.0164
λ_G	0.7262	0.7270	0.6545	0.7268	0.6438	0.7009
a_G	0.0414	0.0206	0.3041	0.0666	0.3065	0.1935
$F'(\rho_e)[eV/\rho_e]$	-5.0429	-4.3559	-1.6946	-5.7437	-1.3236	-4.5747
$F''(\rho_e)\ eV/\rho_e$	1.8945	1.4060	2.5712	2.5341	2.0796	3.9983
$\phi_e\ (eV)$	0.6374	0.5527	0.1509	0.7088	0.0022	0.5411
$\phi_e'\ eV/\overset{0}{A}$	1.3311	1.4349	0.6407	0.9260	0.5196	1.6754
$\phi_e''\ eV/\overset{0\ 2}{A}$	4.0097	3.4668	3.6047	4.2212	3.9128	6.2839
ρ_e	11.5453	17.1253	3.4884	5.1737	2.0780	21.4831
$\rho_e'\left(\rho_e/\overset{0}{A}\right)$	1.5837	1.9765	2.2685	0.9673	2.3553	2.1974
$\rho_e''\left(\rho_e/\overset{0\ 2}{A}\right)$	-0.7849	3.2935	9.6597	-0.6055	10.7060	5.6214
V_{11}/ρ_e	-1.3494	-1.8948	2.2274	-0.7816	2.1971	2.0276

Table 4: Calculated values of the electron density function

	Cu	***Ag***	***Au***	***Ni***	***Pd***	***Pt***
Cu	11.5453	17.4747	24.5771	5.0993	2.3304	23.7185
Ag	12.8573	17.1253	3.6358	6.2043	2.1839	2.2207
Au	21.8770	19.0671	3.4884	9.1400	2.4849	3.6742
Ni	11.5417	17.8859	67.6790	5.1737	2.4223	24.6240
Pd	2.0596	3.6173	8.1268	7.8541	2.0780	4.8639
Pt	17.9264	18.1142	3.5364	8.5635	2.0630	21.4831

Table 5: Calculated values of the pair-potential function

	Cu	***Ag***	***Au***	***Ni***	***Pd***	***Pt***
Cu	0.6371	0.7015	-0.2036	0.6555	0.5792	0.5962
Ag	0.6788	0.5521	0.5232	0.7446	0.5423	0.5306
Au	0.2667	0.1199	0.1509	0.4879	0.1348	-0.0439
Ni	0.7151	0.8026	-0.2289	0.7088	0.7066	0.6615
Pd	-0.0719	-0.0574	-0.1744	0.1012	0.0022	-0.0538
Pt	0.4008	0.5289	0.5579	0.5300	0.5478	0.4511

Table 6: Calculated values for parameters $P_1, P_2, P_3, P_4, P_5, P_6$ *and* P_7

			HOST	**METAL**		
	Cu	***Ag***	***Au***	***Ni***	***Pd***	***Pt***
β	0.532	8.5652	5.8912	8.5652	4.5628	8.5652
P_1	-4.0416	-5.7133	-6.6822	-2.3452	6.5914	6.0673
P_2	-2.0284	-3.3862	40.2019	-1.8756	4.5011	21.4840
P_3	-6.4457e4	6.3573e7	2.607e7	3.6352e^5	1.0536e5	5.9346e6
P_4	-1.3834e6	3.7536e9	1.6048e11	-1.6586e7	-1.5767e8	-1.2903e8
P_5	7.2458e7	7.7005e9	3.415e11	2.4392e8	-4.5929e9	-2.4289e10
P_6	-7.4383e8	6.3819e11	2.9173e12	-1.4583e9	3.9866e9	3.4399e11
P_7	2.2918e9	1.8328e10	8.5944e12	3.0517e9	6.1481e11	3.9903e11

Table 7: Calculated values for parameters $h_1, h_2, h_3, h_4, h_5, h_6$ *and* h_7

		HOST	**METAL**			
	Cu	***Ag***	***Au***	***Ni***	***Pd***	***Pt***
h_1	-5.3294	-7.4658	12.5039	-3.1671	651.0429	8.5499
h_2	1.8454	1.1513	2.2730	17.6402	0.0331	89.0337
h_3	-1.0551e4	5.6868e6	1.43638e8	-1.6591e5	-2.2928e8	-36707e5
h_4	-1.5302e5	3.3456e8	8.8302e9	5.2043e6	3.4090e9	7.1090e6
h_5	1.3435e7	6.8469e9	1.8780e13	-6.0171e7	9.9784e10	1.4857e8
h_6	-1.7423e8	5.6662e10	1.6031e12	3.0388e8	-8.6153e11	-2.0574e9
h_7	6.5180e8	1.6257e11	-4.7210e12	-5.66202e8	-1.3326e13	-2.4038e10

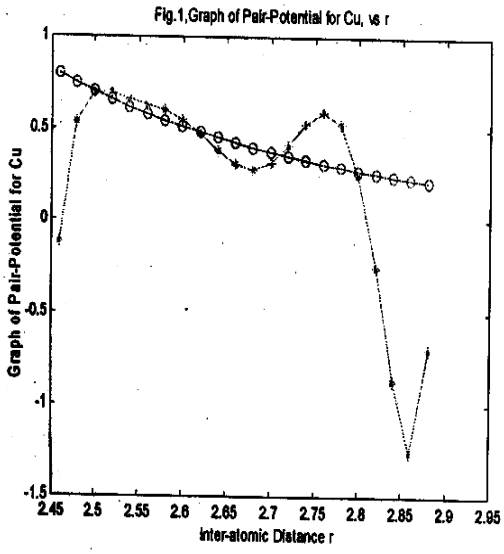
Fig.1,Graph of Pair-Potential for Cu, vs r
Graph of Pair-Potential for Cu
Inter-atomic Distance r

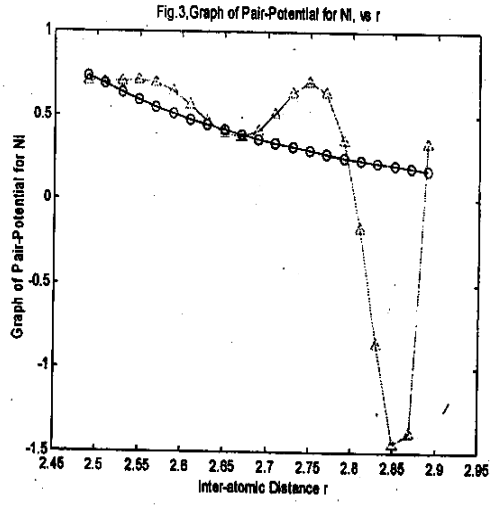
Fig.3,Graph of Pair-Potential for Ni, vs r
Graph of Pair-Potential for Ni
Inter-atomic Distance r

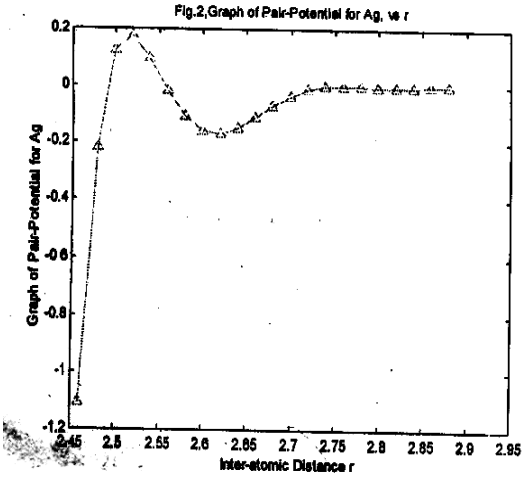
Fig.2,Graph of Pair-Potential for Ag, vs r
Graph of Pair-Potential for Ag
Inter-atomic Distance r

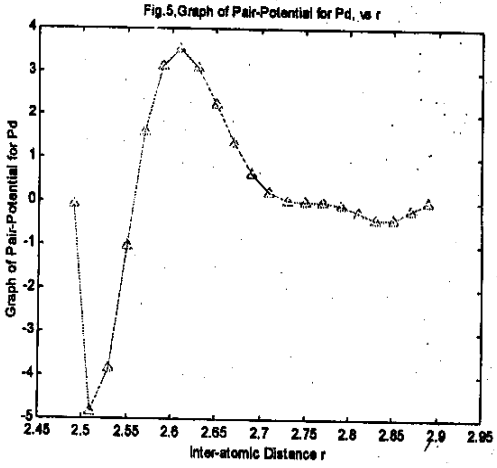
Fig.5,Graph of Pair-Potential for Pd, vs r
Graph of Pair-Potential for Pd
Inter-atomic Distance r

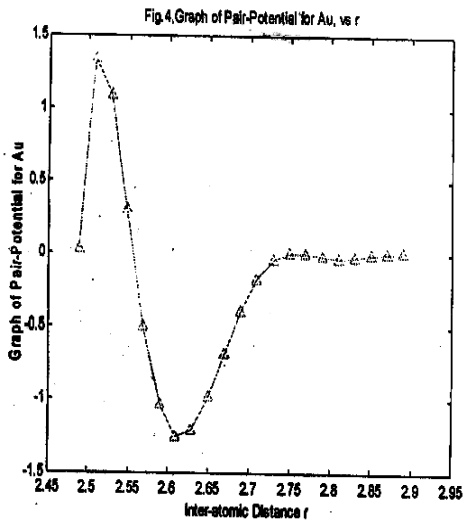
Fig.4,Graph of Pair-Potential for Au, vs r
Graph of Pair-Potential for Au
Inter-atomic Distance r

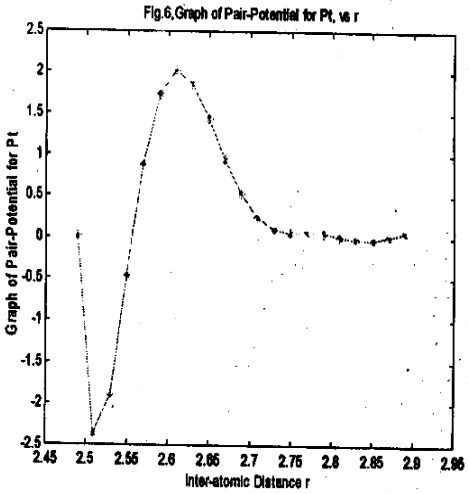
Fig.6,Graph of Pair-Potential for Pt, vs r
Graph of Pair-Potential for Pt
Inter-atomic Distance r

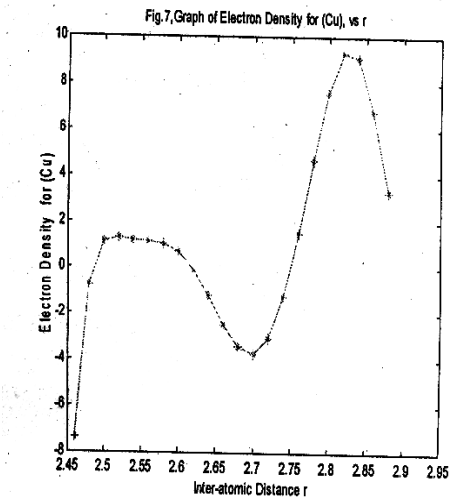
Fig.7,Graph of Electron Density for (Cu), vs r
Electron Density for (Cu)
Inter-atomic Distance r

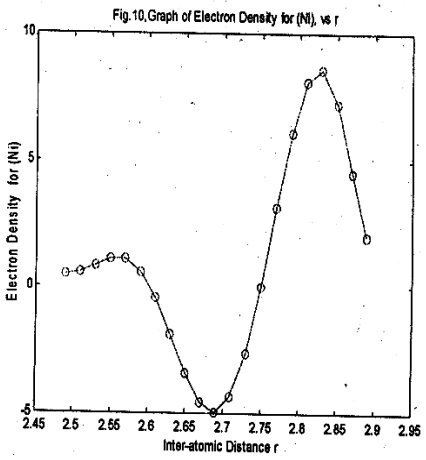
Fig.10,Graph of Electron Density for (Ni), vs r
Electron Density for (Ni)
Inter-atomic Distance r

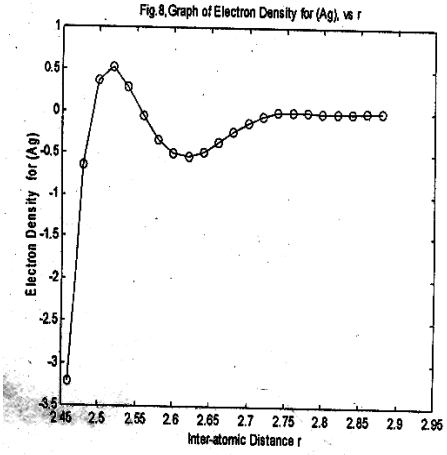
Fig.8,Graph of Electron Density for (Ag), vs r
Electron Density for (Ag)
Inter-atomic Distance r

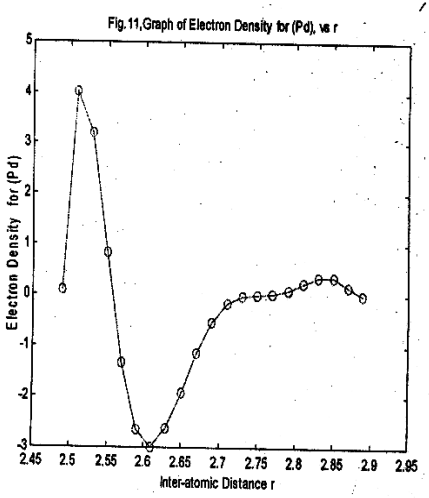
Fig.11,Graph of Electron Density for (Pd), vs r
Electron Density for (Pd)
Inter-atomic Distance r

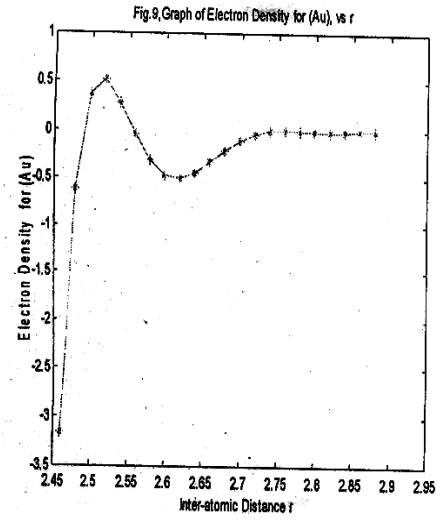
Fig.9,Graph of Electron Density for (Au), vs r
Electron Density for (Au)
Inter-atomic Distance r

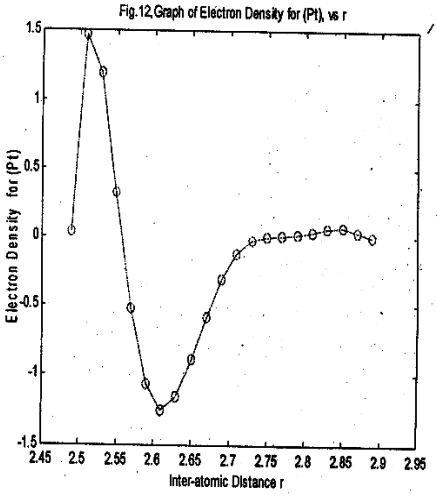
Fig.12,Graph of Electron Density for (Pt), vs r
Electron Density for (Pt)
Inter-atomic Distance r

The curve fits for the analytic functions are shown in figures. 1 - 6 for the electron density and figures 7 – 12 for the pair potential function.

5.0 Conclusion

The problem studied in this paper is that of obtaining appropriate electron density function and a pair potential function for an FCC metal within the embedded atom method (EAM). The approach adopted is to use the experimental dilute limit heats of solution of the binary alloys of FCC metals as input parameters into Johnson's analytical model for calculating the dilute limit heats of solution, and to try to determine the needed functions consistently. Both the curve fit and actual numerical values obtained for the electron density function and pair potential function satisfy Johnson's equation for the dilute limit heats of solution and also the EAM equations. However, the functions obtained do not support the assumption generally made of a single exponential function of r for the electron density function and the pair potential function.

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