

On the Modified Embedded Atom Method for Strontium: A New Algorithmic Approach

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Abstract

In this paper we derive an expression for the embedding energy as a function of the background electron density using the physical interpretation of its slope and curvature at equilibrium and beyond. The total energy expansion in rapidly convergent series allows the characterization of the embedding energy function $F(\rho)$ by a second-order ordinary differential equation. Our modeled $F(\rho)$ captures the essential physics while maintaining simplicity - a quality which endows the embedded atom method (EAM) and concomitantly the modified embedded atom method (MEAM) with excellent numerical efficiency. Preliminary investigations of the parameters of Strontium attest to the validity of our theoretical model.

Keywords: EAM, MEAM and embedding energy function $F(\rho)$.

1.0 Introduction

The modified embedded atom method (MEAM) is an offshoot of the embedded atom method (EAM) introduced by Daw and Baskes [1]. EAM and by extension, MEAM are commonly used to calculate the ground state properties of real metals. A detailed understanding of the energies in non-periodic structures like point defects, alloys, vacancies, impurities, surface phenomena etc. have been dealt with successfully by these models. The original model, EAM is based on the density functional theory (DFT) which incorporates many-body interactions while requiring some experimental quantities as input; it is computationally fast.

Daw and Baskes [1] gave a heuristic derivation using DFT and came up with an ansatz that

$$E_{cohesive} = \sum_i F_i \left(\sum_{j \neq i} \rho_j^a(r_{ij}) \right) + \frac{1}{2} \sum_{i,j} \phi_{ij}(r_{ij}) \quad (1.1)$$

In Eq(1.1), $F(\rho)$ represents the embedding energy function, ρ^a is the spherical averaged atomic density and ϕ is an electrostatic two-body interaction. The host electron density, assumed to be a linear superposition of contributions from individual atoms, is defined through equation

$$\rho = \sum_{j \neq i} \rho_j^a(r_{ij}) \quad (1.2)$$

Eq.(1.1) is known for computational simplicity which adequately caters for defects and other physical phenomena in solid or liquid state of metal. So far, EAM features three important functions which are $F(\rho)$, $\rho(r)$ and $\phi(r)$.

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The embedding energy function $F(\rho)$ is universal and is independent of host; its form is unknown and thus any choice is an approximation. The form of $F(\rho)$ adopted by Daw and Baskes [1, 2] in their calculations was determined by a complex fitting procedure. It is important to state that $F(\rho)$ and $\phi(r)$ are not uniquely determined by empirical or theoretical procedure. For example, Daw [3] adopted an EAM model that utilized the Thomas-Fermi-Dirac-von Weizsäcker approach for the kinetic energy with local exchange and correlation and frozen-electron distributions.

Despite the great successes recorded by EAM, it is plagued by some limitations. A particular drawback is its lack of angular forces or directional bonding. An attempt to improve EAM led to the Modified Embedded Atom Method (MEAM) [4]. The major difference between EAM and MEAM depends on the choice of the electron density $\rho(r)$. Thus, in EAM $\rho(r)$ has spherical symmetry while in MEAM $\rho(r)$ incorporates the s, p, d, f symmetries.

Although various modifications have been made in EAM leading to MEAM, there still exist the problems of lack of transferability, overestimation of monovacancy formation energies for some materials, non-applicability to materials with $c_{12} - c_{44} < 0$ among others. The various shortcomings point to the fact that some MEAM models are not valid. To ease out some of these problems we propose an embedding energy function which is deeply rooted in the perturbation theory of quasiatoms and density functional theory as pointed out by Stott and Zaremba [5] while incorporating the recommendation of first-principle calculations for a consistent embedding energy function.

The remaining part of this paper is organized as follows: Section 2 surveys briefly the popular embedding energy functions in literature with a view to analyzing their physical and theoretical structures; the new embedding energy function is formulated in section 3 while the preliminary results and findings on Strontium are presented in section 4 having tested our $F(\rho)$. Finally, section 5 concludes the work.

2.0 Existing models

Usually the functional form of the embedding energy function is unknown. The information about $F(\rho)$ for densities well away from the equilibrium value may be obtained through the universal equation of Rose *et al* [6]; it is an empirical equation of state of the expanded (or compressed) metal for which the electron density at each lattice site is substantially different from its equilibrium value. It is given by

$$E_s = -E_c \left[1 + \alpha \left(\frac{r}{r_0} - 1 \right) \right] \exp \left[-\alpha \left(\frac{r}{r_0} - 1 \right) \right] \quad (2.1)$$

where

$$\alpha^2 = \frac{9\Omega B}{E_c} \quad (2.2)$$

B is the bulk modulus, E_c is the cohesive energy, r_0 is the nearest-neighbour or equilibrium distance and Ω is the atomic volume. Total energy $E_{tot} = NE_s$ and N is the number of atoms. In some early versions of EAM and MEAM [7, 8], $F(\rho)$ was uniquely defined by a requirement that the total energy of the homogeneous solid be related to the universal equation of state (Eq.(2.1)) such that

$$E_s = F(\rho(r)) + \frac{1}{2} \sum_m \phi(r_m) \quad (2.3)$$

where

$$\rho(r) = \sum_m f(r_m) \quad (2.4)$$

and

$$\Phi(r) = \frac{1}{2} \sum_m \phi(r_m) \quad (2.5)$$

$F(\rho(r))$ is the energy to embed atom i in $\rho_{h,i}$ which is the host electron density at atom i due to all other atoms. Function $f(r_j)$ is the electron density at atom j as a function of distance from its centre. Therefore the embedding energy function as a function of r is

$$F(r) = -E_c \left[1 + \alpha \left(\frac{r}{r_0} - 1 \right) \right] \exp \left[-\alpha \left(\frac{r}{r_0} - 1 \right) \right] - \phi(r) \quad (2.6)$$

A particular EAM version by Johnson [8] used an electronic density of form

$$f(r) = f_0 \exp \left[-\beta \left(\frac{r}{r_0} - 1 \right) \right], \quad r \leq r_c \quad (2.7)$$

and a Born-Mayer potential of form

$$\phi(r) = \phi_0 \exp \left[-\gamma \left(\frac{r}{r_0} - 1 \right) \right], \quad r \leq r_c \quad (2.8)$$

Substituting Eqs.(2.7) and (2.8) into Eq.(2.6) yields

$$F(r) = -E_c \left[1 + \alpha \left(\frac{r}{r_0} - 1 \right) \right] \exp \left[-\alpha \left(\frac{r}{r_0} - 1 \right) \right] - \phi_0 \exp \left[-\gamma \left(\frac{r}{r_0} - 1 \right) \right] \quad (2.9)$$

Note that r_c is the cut-off parameter between 1st and 2nd neighbours. To write $F(r)$ as $F(\rho)$, Eq.(2.7) must be inverted to give

$$\rho(r) = \rho_0 \exp \left[-\beta \left(\frac{r}{r_0} - 1 \right) \right] \quad (2.10)$$

which implies

$$-\frac{1}{\beta} \ln \frac{\rho}{\rho_0} = \left(\frac{r}{r_0} - 1 \right) \quad \text{or} \quad \ln \left(\frac{\rho}{\rho_0} \right)^{\frac{\alpha}{\beta}} = -\alpha \left(\frac{r}{r_0} - 1 \right) \quad (2.11a)$$

leading to

$$\left(\frac{\rho}{\rho_0} \right)^{\frac{\alpha}{\beta}} = \exp \left[-\alpha \left(\frac{r}{r_0} - 1 \right) \right] \quad (2.11b)$$

Also from Eq.(2.10)

$$\left(\frac{\rho}{\rho_0} \right)^{\frac{\gamma}{\beta}} = \exp \left[-\gamma \left(\frac{r}{r_0} - 1 \right) \right] \quad (2.11c)$$

By substituting Eqs.(2.11a, b & c) into Eq.(2.9) one obtains [8]

$$F(\rho) = AE_c \left[\frac{\alpha}{\beta} \ln \left(\frac{\rho}{\rho_0} \right) - 1 \right] - \phi_0 \left(\frac{\rho}{\rho_0} \right)^{\frac{\gamma}{\beta}} \quad (2.12)$$

where

$A = \left(\frac{\rho}{\rho_0} \right)^{\frac{\alpha}{\beta}}$, α , β and ϕ_0 are the fitting parameters. Note that α may be calculated from Eq.(2.2).

A basic limitation of EAM is that it spherically averages the electron density which precludes directional bonding. Baskes [4] adopted a modified embedded atom method (MEAM) of form

$$F(\rho) = AE_c \frac{\rho}{\rho_0} \ln \left(\frac{\rho}{\rho_0} \right) \quad (2.13)$$

Eq.(2.13) has A as a fitting parameter and ρ_0 as a density scaling parameter which is assumed to be the density in the equilibrium reference structure. Eq.(2.13) is believed to include directional bonding. Thus at a particular atom the mean-square density is given by

$$\bar{\rho}^2 = \sum_{h=0}^3 t^{(h)} \rho^{(h)2} \quad (2.14)$$

where $h = 0, 1, 2, 3$ correspond to s, p, d and f symmetries respectively.

Yuan *et al* [9] modified Eq.(2.13) further by introducing a new adjustable parameter K to the embedding energy function to take care of the problem encountered in the calculation of the surface energy of *bcc* Lithium. It is simply given by

$$F(\rho) = AE_c \left[\frac{\rho}{\rho_0} \ln \left(\frac{\rho}{\rho_0} \right) - K \right] \quad (2.15)$$

Eq.(2.15) still suffers non-transferability when applied to *bcc* Vanadium where it overestimates the monovacancy formation energy by 50%.

Yet another model purportedly fashioned to correct the shortcoming of Eq.(2.15) and to take care of both positive and negative curvatures of the embedding energy function (Cauchy-Discrepancy) is the one suggested by Oni-Ojo *et al* [10] given by

$$F(\rho) = AE_c \left(\frac{\rho}{\rho_0} \right)^{\lambda} \left[\ln \left(\frac{\rho}{\rho_0} \right)^{\alpha} - K \right] \quad (2.16)$$

where A, λ, α and K are the adjustable parameters. Eq.(2.16) was formulated to satisfy a second-order ordinary differential equation of form

$$\frac{d^2 F}{d\rho^2} - \frac{\gamma_1}{\rho} \frac{dF}{d\rho} + \frac{\gamma_0}{\rho} F = 0 \quad (2.17)$$

with provisos

$$\gamma_0 = \lambda\gamma_1 - \lambda^2 + \lambda \quad \text{and} \quad \gamma_1 = 2\lambda - 1 \quad (2.18)$$

3.0 Formulation of a new embedding energy function

The goal here is to derive an embedding energy function which is an explicit function of the electronic density of the metal that is very simple to evaluate. Our approach relies on the attributes of $F(\rho)$ that it possesses a single minimum and be linear at higher densities. To make the zero of energy correspond to neutral atoms separated by infinite distances, $F(\rho)$ is constrained to go to zero at vanishing electron density.

If $F(\rho)$ is completely linear, its contribution can only be attributed to the action of a two-body potential. Thus it is the curvature of $F(\rho)$ that accounts for the many-body or local-volume effect of EAM and MEAM and hence its non-linear nature. Since pair potentials alone cannot represent adequately the elastic properties of real solids, we shall take care of the nonlinearity of $F(\rho)$ through the curvature of $F(\rho)$ at equilibrium.

Analytical expression can be assigned to $F(\rho)$ if we are mindful of the fact that:

- i. The slope of $F(\rho)$ does not depend on the bulk modulus or the cohesive energy and that the curvature ($d^2F/d\rho^2$) is quite small.
- ii. The unrelaxed vacancy-formation energy involves changes in energy near equilibrium and thus it is dominated by the slope of $F(\rho)$. That is, the shear modulus rather than the bulk modulus (or the cohesive energy) is the dominant parameter in determining the unrelaxed vacancy-formation energy.
- iii. The unrelaxed divacancy-binding energy and the unrelaxed surface energy contain terms which depend on $F(\rho)$ at the electron densities which are significantly smaller than the equilibrium electron density ρ_0 . This is an indication that the curvature plays a larger role here while the shear modulus does not.

Thus, by using a perturbation expansion for the inhomogeneous background density, the total energy of a quasiautom can be expressed as a function of the background density and its gradient.

The first-principle calculations also reveal information about the general behavior of $F(\rho)$ as follows:

- i. The embedding energy (defined relative to the free-atom energy) must go to zero for zero electron density, have a negative slope and a positive curvature for the background electron densities found in metal.
- ii. The pair-interaction must be repulsive.

If the energies of these quantities are expanded in rapidly convergent series, the lowest-order terms in the expansion depend on the slope of $F(\rho)$ at the equilibrium electron density and consequently do not depend on either the bulk modulus or the cohesive energy. Hence, we write (Taylor's expansion about $\rho = 0$)

$$E(\rho) = E(0) + \rho E'(0) + \frac{1}{2} \rho^2 E''(0) + \dots \quad (3.1)$$

We shall identify the following:

- i. $E(0) \rightarrow \phi_0$ (zero of energy) and $F(0) \rightarrow 0$
- ii. $E'(0) \rightarrow -\frac{dF}{d\rho} \neq 0$ due to non-linearity effect
- iii. $E''(0) \rightarrow \frac{d^2F}{d\rho^2}$ via $c_{12} - c_{44}$
- iv. $E(\rho) \rightarrow (\phi_0 + F(\rho))$

As a result, Eq.(3.1) yields

$$F''(0) - \frac{a}{\rho} F'(0) + \frac{b}{\rho^2} F(\rho) = 0 \quad (3.2)$$

where a and b are constants to be determined. Eq.(3.2) is the so called Cauchy-Euler equation [11, 12]. It has a power series solution (Frobenius method) of form

$$F(\rho) = \sum_{m=0}^{\infty} C_m \rho^{m+q}, \quad q > 0 \quad (3.3)$$

In Eq.(3.3), C_m are the constant coefficients. Substituting Eq.(3.3) into Eq.(3.2) produces the indicial equation given by

$$q^2 - (1+a)q + b = 0 \quad (3.4)$$

with solution

$$q_{1,2} = \frac{(1+a) \pm \sqrt{(1+a)^2 - 4b}}{2} \quad (3.5)$$

We recognize the fact that

$$q_1 - q_2 = \begin{cases} \text{integer} \\ 0 \\ \text{non-integer} \end{cases} \quad (3.6)$$

Eq.(3.6) plays a major role in shaping the functional form of $F(\rho)$. Whatever the nature of $q_1 - q_2$ we shall choose a solution of Eq.(3.2) of form

$$F(\rho) = C\rho^{q_1} + D\rho^{q_2} \ln \rho \quad (3.7)$$

where C and D are the arbitrary constants. For example, if $q_1 = q_2 = 1$ and $C = 0$ we shall recover the popular $F(\rho)$ of Baskes [4] given by

$$\begin{aligned} F(\rho) &= -AE_0 \rho \ln \rho, \quad D = -AE_0 \\ &= -AE_0 \left(\frac{\rho}{\rho_0} \right) \ln \left(\frac{\rho}{\rho_0} \right) \end{aligned} \quad (2.12)$$

where ρ_0 is a density scaling parameter. We propose an embedding energy function given by the functional form

$$F(\rho) = AE_0 \left(\frac{\rho}{\rho_0} \right)^{q_1} - AE_0 \left(\frac{\rho}{\rho_0} \right)^{q_2} \ln \left(\frac{\rho}{\rho_0} \right), C = -D = AE_0 \quad \forall \quad q_1 - q_2 \neq 0 \quad (3.8)$$

where A, q_1 and q_2 are the adjustable parameters subject to

$$a \geq 2\sqrt{b} - 1 \quad (3.9)$$

Eq.(3.8) yields $F(\rho_0) = AE_0$ and $F(0) = 0$ as it should unlike Eq.(2.12) which is not physical at $\rho = \rho_0$.

Though Eq.(2.17) and Eq(3.2) are essentially the same, our approach at formulating Eq(3.2) is somewhat different because of its sound theoretical foundation culminating in a simple explicit expression (Eq.(3.8)) for $F(\rho)$. The derivation of Eq.(3.2) is devoid of any arbitrariness.

4.0 Calculation Procedure: Application to the *fcc* lattice

To test our simple analytic model (Eq.(3.8)), we performed simple nearest-neighbour analytic calculations for *fcc* lattices. The essential equations for our calculations are:

$$F(\rho) = AE_0 \left(\frac{\rho}{\rho_0} \right)^{q_1} - AE_0 \left(\frac{\rho}{\rho_0} \right)^{q_2} \ln \left(\frac{\rho}{\rho_0} \right) \quad (3.8)$$

$$F(\rho_0) = AE_0 \quad \text{in units of eV} \quad (4.1)$$

Thus,

$$F'(\rho_0) = \frac{AE_0}{\rho_0} (q_1 - 1) \quad (4.2)$$

$$F''(\rho_0) = \frac{AE_0}{\rho_0^2} [q_1^2 - q_1 - 2q_2 + 1] \quad (4.3)$$

For nearest-neighbour contribution, Eq.(2.4) and Eq.(2.5) yield

$$\rho(r_1) = 12\rho_0(r_1) \quad (4.6)$$

$$\Phi(r_1) = 6\phi(r_1) \quad (4.7)$$

The energies of monovacancy, divacancy, planar-surface formations etc. for the *fcc* metals are dominated by the contributions before relaxation. These energies are readily calculated from their analytic expressions via Eq.(3.8) if q_1 and q_2 are known. The monovacancy formation energy is

$$E_{mf} = -12E_{12} + 12E_{11} \quad (4.8)$$

where

$$E_n = F\left(\frac{n}{12}\rho_0\right) + \frac{n}{12}\phi_0 \quad (4.9)$$

$$E_{12} = E_0 = -E_c \quad \text{and} \quad F(\rho_0) = E_0 - \phi_0 = AE_0 \quad (\text{in our case}) \quad (4.10)$$

where E_0 is the total energy per atom while E_c is the cohesive energy.

Therefore,

$$E_{mf} = 12F\left(\frac{11}{12}\rho_0\right) - E_0(1 + 11A) \quad (4.11)$$

The surface energies are

$$\Gamma_{100} = \frac{2}{a^2} (E_8 - E_{12}) = \frac{2}{a^2} \left\{ F\left(\frac{8}{12}\rho_0\right) - \frac{1}{3}E_0(1 + 2A) \right\} \quad (4.12)$$

$$\Gamma_{110} = \frac{\sqrt{2}}{a^2} (E_7 + E_{11} - 2E_{12}) = \frac{\sqrt{2}}{a^2} \left\{ F\left(\frac{7}{12}\rho_0\right) + F\left(\frac{11}{12}\rho_0\right) - \frac{1}{2}E_0(1 + 3A) \right\} \quad (4.13)$$

$$\Gamma_{111} = \frac{4}{a^2\sqrt{3}} (E_9 - E_{12}) = \frac{4}{a^2\sqrt{3}} \left\{ F\left(\frac{9}{12}\rho_0\right) - \frac{1}{4}E_0(1 + 3A) \right\} \quad (4.14)$$

From Eq.(3.8):

$$F\left(\frac{7}{12}\rho_0\right) = AE_0 \left(\frac{7}{12} \right)^{q_1} - AE_0 \left(\frac{7}{12} \right)^{q_2} \ln \left(\frac{7}{12} \right) \quad (4.15)$$

$$F\left(\frac{8}{12}\rho_0\right) = AE_0 \left(\frac{8}{12} \right)^{q_1} - AE_0 \left(\frac{8}{12} \right)^{q_2} \ln \left(\frac{8}{12} \right) \quad (4.16)$$

$$F\left(\frac{9}{12}\rho_0\right) = AE_0 \left(\frac{9}{12} \right)^{q_1} - AE_0 \left(\frac{9}{12} \right)^{q_2} \ln \left(\frac{9}{12} \right) \quad (4.17)$$

$$F\left(\frac{11}{12}\rho_0\right) = AE_0 \left(\frac{11}{12} \right)^{q_1} - AE_0 \left(\frac{11}{12} \right)^{q_2} \ln \left(\frac{11}{12} \right) \quad (4.18)$$

We shall make use of the following series expansions in Eqs.(4.15 – 4.18):

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots \dots \dots \quad (4.19)$$

$$(1+x)^n = 1 + \frac{nx}{1!} + \frac{n(n-1)x^2}{2!} + \dots \quad (4.20)$$

Thus,

$$F\left[\left(1 - \frac{n}{12}\right)\rho_0\right] = AE_0 \left\{ \begin{array}{l} 1 + \frac{n}{12} \left[1 + \frac{1}{2} \left(\frac{n}{12}\right) + \frac{1}{3} \left(\frac{n}{12}\right)^2 + \frac{1}{4} \left(\frac{n}{12}\right)^3 + \frac{1}{5} \left(\frac{n}{12}\right)^4 + \dots \right] \\ - \frac{n}{12} \left[1 + \frac{1}{2} \left(\frac{n}{12}\right) + \frac{1}{3} \left(\frac{n}{12}\right)^2 + \frac{1}{4} \left(\frac{n}{12}\right)^3 + \frac{1}{5} \left(\frac{n}{12}\right)^4 + \dots \right] q_1 \\ + \frac{1}{2} \left(\frac{n}{12}\right)^2 \left[1 + \frac{1}{2} \left(\frac{n}{12}\right) + \frac{1}{3} \left(\frac{n}{12}\right)^2 + \frac{1}{4} \left(\frac{n}{12}\right)^3 + \frac{1}{5} \left(\frac{n}{12}\right)^4 + \dots \right] q_1^2 \\ - \frac{1}{3!} \left(\frac{n}{12}\right)^3 \left[1 + \frac{1}{2} \left(\frac{n}{12}\right) + \frac{1}{3} \left(\frac{n}{12}\right)^2 + \frac{1}{4} \left(\frac{n}{12}\right)^3 + \frac{1}{5} \left(\frac{n}{12}\right)^4 + \dots \right] q_1^3 \\ - \left(\frac{n}{12}\right)^2 \left[1 + \frac{1}{2} \left(\frac{n}{12}\right) + \frac{1}{3} \left(\frac{n}{12}\right)^2 + \frac{1}{4} \left(\frac{n}{12}\right)^3 + \frac{1}{5} \left(\frac{n}{12}\right)^4 + \dots \right]^2 q_2 \\ + \frac{1}{2} \left(\frac{n}{12}\right)^3 \left[1 + \frac{1}{2} \left(\frac{n}{12}\right) + \frac{1}{3} \left(\frac{n}{12}\right)^2 + \frac{1}{4} \left(\frac{n}{12}\right)^3 + \frac{1}{5} \left(\frac{n}{12}\right)^4 + \dots \right]^2 q_2^2 \\ - \frac{1}{3!} \left(\frac{n}{12}\right)^4 \left[1 + \frac{1}{2} \left(\frac{n}{12}\right) + \frac{1}{3} \left(\frac{n}{12}\right)^2 + \frac{1}{4} \left(\frac{n}{12}\right)^3 + \frac{1}{5} \left(\frac{n}{12}\right)^4 + \dots \right]^2 q_2^3 \end{array} \right\} \quad (4.21)$$

where

$$F\left(\frac{7}{12}\rho_0\right) = F\left[\left(1 - \frac{5}{12}\right)\rho_0\right] \quad (4.22)$$

$$F\left(\frac{8}{12}\rho_0\right) = F\left[\left(1 - \frac{4}{12}\right)\rho_0\right] \quad (4.23)$$

$$F\left(\frac{9}{12}\rho_0\right) = F\left[\left(1 - \frac{3}{12}\right)\rho_0\right] \quad (4.24)$$

$$F\left(\frac{11}{12}\rho_0\right) = F\left[\left(1 - \frac{1}{12}\right)\rho_0\right] \quad (4.25)$$

The required experimental parameters are E_0 , E_{mf} and lattice constant a .

5.0 Results and Discussion

To test the reliability of our model, we calculated numerically the surface energies along the three different orientations and for ease of comparison chose Strontium as a prototype. We adjusted q_1 , q_2 and A to match the experimental value of the monovacancy formation energy E_{mf} . Our algorithm was based on a very simple procedure which utilized 1000 numerical grid points with spacing such that $\Delta A = \Delta q_1 = \Delta q_2 = 10^{-5}$. Thus values $q_1 = 0.561$, $q_2 = 2.522$ and $A = 0.515$ fitted Eq.(4.11) with $E_{mf} = 0.600\text{eV}$ perfectly. Subsequently, these 3 parameters were used in Eqs.(4.12-4.14) to calculate the unrelaxed surface energies. The results, compared to the first principle calculations, other MEAM results and experimental data of deBoer *et al* [13] are presented in Table 1. The first 3 entries are the input parameters taken from Kittel [14].

Table 1: MEAM results for Strontium using Eq.(3.8) compared to other theoretical calculations and experiment where available.

Quantity		d			
Lattice constant (a)		6.08Å			
Cohesive energy (E_c)		1.72eV			
Monovacancy formation energy (E_{mf})		0.600eV			
Surface energy (ergs/cm ²)	Present work	a	b	c	
$\Gamma(100)$	310.603	355.000		408.000	
$\Gamma(110)$	496.053	368.000	432.000		
$\Gamma(111)$	225.849	277.000	287.000	428.000	410.000

a: Equivalent crystal theory calculation [15]

b: First principle calculation [16]

c: First principle calculation [17]

d: Experiment [13]

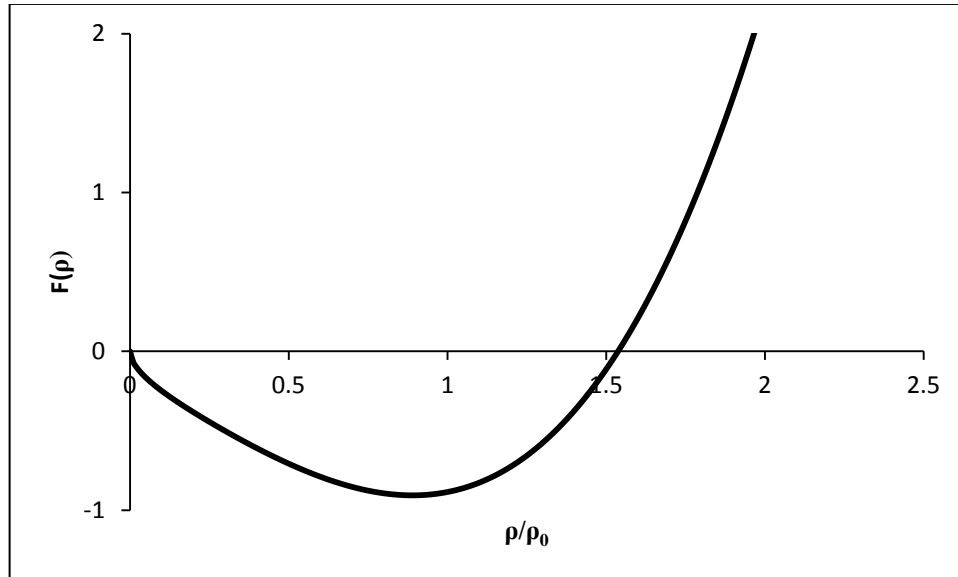


Figure 1: Embedding energy function for Strontium (present work).

The embedding function $F(\rho)$ (Eq(3.8)) plotted for Strontium was displayed in Fig.1. Our $F(\rho)$ has the desired behavior: a simple minimum at lower densities and a nearly linear upward slope at higher densities. It should be mentioned that convergence was very good in all the series considered and results definitely improved with the number of terms used. Our result for $\Gamma(111)$ deviates a bit from experiment but it is realistic. We are aware of the fact that the available first principle results and experimental data are generally uncertain. It is well known that various groups predict or measure different values for the same material.

6. Conclusion

The purpose of the present work was to capture the essence of MEAM by taking into consideration the physical interpretation of each term involved in the total energy of a metal. Thus, we developed a near-analytic model for the embedding energy of a metal which reproduced very well some important features of the metals. The physical experimental inputs of our model were very few which gave it an edge over other MEAM models. They were the lattice constant, cohesive energy and the vacancy formation energy.

The preliminary results obtained for Strontium compared favourably with the available experimental and other theoretical results. Our calculated data for Strontium revealed that the first derivative (shear modulus) rather than the second derivative (bulk modulus) of the embedding energy function dominated the value recorded for vacancy formation energy. On the other hand, the curvature of the embedding energy function accounted for the many-body aspect of MEAM.

It should be stated that our calculation did not make use of the explicit form of the inter-atomic potential, instead ϕ_0 was subsumed into A . This is to say that our model is not constrained in any way by the specific form of the MEAM potential. Whatever the form of the MEAM potential, one can always find a means of incorporating it and other correlation functions into the model for better accuracy.

To appreciate the genuineness of our model, we have already applied Eq.(3.8) to several *bcc* and *fcc* metals. The agreements with experiments were found to be generally good. More detailed results shall be published soon. For further work, we are considering an extension to *hcp* metals and the inclusion of a background atomic density ρ_0 which is angular and reference-state dependent. We are also considering incorporating electron correlations via density-gradient corrections.

References

- [1] Daw M. S. and Baskes M. I., "A semi-empirical quantum mechanical calculation of Hydrogen embrittlement in metals", *Phys. Rev. Lett.*, Vol.50, № 17, pp.1285-1288, 1983.
- [2] Daw M. S. and Baskes M. I., "Derivation and application to impurities, surfaces and other defects in metals", *Phys. Rev. B*, Vol.29, № 12, pp.6443-6453, 1984.
- [3] Daw M. S., "Model of metallic cohesion: The embedded-atom method", *Phys. Rev. B*, Vol. 39, № 11, pp. 7441-7451, 1989.
- [4] Baskes M. I., "Modified Embedded-Atom Potentials for Cubic Materials and Impurities" *Phys. Rev. B*, Vol. 46, № 5, pp. 2727-2742, 1992.
- [5] Stott M. J. and Zaremba E., "Quasiatoms: An approach to atoms in non-uniform electronic systems", *Phys. Rev. B*, Vol.22, № 4, pp.1564-1583, 1980.

- [6] Rose J. H., Smith J. R., Guinea F. and Ferrante J., “Universal Features of the Equation of State of Metals”, *Phys. Rev. B*, Vol.29, № 6, pp.2963-2969, 1984.
- [7] Foiles S. M., Baskes M. I. and Daw M. S., “Embedded-atom-method functions for the fcc metals Cu, Ag, Ni, Pd, Pt and their alloys”, *Phys. Rev. B*, Vol. 33, № 12, pp. 7983-7991, 1986.
- [8] Johnson R. A., “Analytic nearest-neighbor model for fcc metals”, *Phys. Rev. B*, Vol.37, № 8, pp. 3924-3921, 1988.
- [9] Yuan X, Takahashi K., Yin Y. and Onzawa T, “Development of MEAM for a bcc metal: lithium”, *Modeling Simul. Mater. Sci. Eng.* Vol.11, № 4, pp. 447-456, 2003.
- [10] Oni-Ojo A., Aghemenloh E. and Idiodi J.O.A., “On recent development on the embedded atom method” *J. Nig. Assoc. Math. Phys.* Vol. 9, pp. 507-512, 2005.
- [11] Kreyszig E., “Advanced Engineering Mathematics”, *Wiley Eastern Limited, 5th ed., printed in India*, Ch. 4, pp. 161-163, 1988.
- [12] Riley K. F., Hobson M. P. and Bence S. I., “Mathematical Methods for physics and engineering”, *Cambridge University Press, Low price edition*, Ch. 13, pp. 437-439, 1999.
- [13] deBoer F. R., Boom R., Mattens W. C. M., Miedema A. R. and Niessen A. R., “Cohesion in metals; Transition metal alloys”, North-Holland, Amsterdam, 1988.
- [14] Kittel C., “Introduction to Solid State Physics”, *Wiley Eastern Limited, 5th ed., printed in India*, Ch. 1, pp. 31, Ch.3, pp.74, 1985.
- [15] Aghemenloh E. and Idiodi J. O. A. “Equivalent crystal theory of fcc metal surfaces”, *J. Nig. Ass. Math Phys.*, Vol.2, pp. 271-284, 1998.
- [16] Skriver H. L. and Rosengaard N. M., “Surface energy and work function of metals”, *Phys. Rev. B*, Vol.46, № 11, pp. 7157-7168, 1988.
- [17] Vitos L., Ruban A. V., Skriver H. L. and Kollar J., “The surface energy of metals”, *Surf. Sci.*, Vol.411, pp. 186-202, 1998.