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Comparison of Inter-atomic Pair Potential Curves of different GEAM iterated values for Sr and Ir

***Oni-Ojo A. A. and Aiyohuyin E. O.**

Department of Physics, University of Benin, Benin City, Nigeria

*Corresponding author's email: amenaghawon.oni-ojo@uniben.edu

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ABSTRACT

In this study, the inter-atomic pair potential curve of Sr and Ir are compared with the potential curve of Rose et al. (1984) using the values predicted in our earlier study (The surface energy calculation for fcc metals with negative Cauchy's discrepancy using the GEAM), utilizing an EAM model developed by Oni-Ojo et al. (2007) that ha demonstrated efficacy in predicting the low index surface energies of Sr and Ir, both of which have negative Cauchy's discrepancy.

INTRODUCTION

Within the embedded - atom method (EAM) introduced by Daw and Baskes (1983 and 1984), which was successful in predicting several properties of metals such as: face-centred cubic (fcc), body-centered cubic (bcc), and diamond structures (Daw and Baskes, 1984, Adams and Foiles, 1990, Baskes et al, 1989, Baskes, 1992, Smith and Banejea, 1987, Foiles et al. 1986, Johnson, 1988), came other models: the modified embedded-atom method (MEAM), Baskes et al. (1989) and Baskes (1992), the analytical embedded atom method (AEAM) Johnson (1988) and Johnson and Oh (1988 and 1989), and the modified analytical embedded atom method (MAEAM), Wen and Zhang (1987 and 1988) all of which tried to improve on the original EAM just the Generalized embedded atom method (GEAM) designed by Oni-Ojo et al. (2007).

The GEAM since its inception has been able to predict the low-index surface energies of fcc and bcc metals that are in good agreement with the average experimental values using iterated parameters values Oni-Ojo (2011) and Oni-Ojo et al. (2007, 2015, 2023[a] and 2023[b]). As a focus in this study, we investigate the pair potential curve of Sr and Ir using GEAM parameters' values as reported in our preceding paper in this very edition: Surface Energy Calculation for fcc metals with negative Cauchy's discrepancy using the GEAM.

MATERIALS AND METHODS

In the GEAM, we have modified the embedding function of Yuan et al. (2003) to produce four parameters generalized embedding function $F(\rho)$.

$$F(\rho) = AE_0\left({}^{\rho}/_{\rho_0}\right)^{\lambda}\left[\ln\left({}^{\rho}/_{\rho_0}\right)^{\alpha} - k\right] \qquad (1)$$

Where, A, λ, α and K are the GEAM parameters that provide flexibility to the model. Like every other model of the EAM, the total energy of a system in the GEAM, E_{tot} is approximated to be, the sum total of the embedding and the pair potential function.

$$E_{tot} = \sum_{j\neq i} F_i\left(\rho_{h,i}\right) + \frac{1}{2}\sum \phi_{i,j}(R_{i,j}) \qquad (2)$$

where $F(\rho)$ denotes the embedding function, that is, the energy required to immerse an atom in the background electron density $\rho(R)$ at site i, and $\phi_{i,j}(R)$ denotes the screened pair potential between atoms i and j.

In practice, functional forms are chosen for $F_i\left(\rho_{h,i}\right)$ and $\phi_{i,j}$ in equation (2) and the parameters in each of these functions are determined by fitting to a limited set of bulk properties.

For the density function $\rho(R)$, this work adopted a simple density function of the form that can be seen in other EAM,

$$\rho(R) = \rho_e . e^{-\beta.\left(\frac{r}{r_0}-1\right)} \qquad (3)$$

β is a parameter needed to fit the density function $\rho(R)$. For the pair potential, a 3-parameter model is adopted, which for large R is dominated by Johnson and Oh's (1988) exponentially decreasing function;

$$\phi_{i,j}(R) = B_1 . e^{-P.\left(\frac{r}{r_0}-1\right)} + B_2 . e^{-P.\left(\frac{2}{\sqrt{3}}\frac{r}{r_0}-1\right)} \qquad (4)$$

Where B_1, B_2 and P, are parameters that must be determined to fit the electrostatics pair potential $\phi_{i,j}(R)$, By demanding that equation (1) satisfy and reproduce the mono-vacancy formation energy E_{iv}^{f} ,

$$E_{iv}^{f} = 12F\left(\frac{11}{12}\rho_0\right) - 11F(\rho_0) - U_0 \qquad (5)$$

gives

$$\lambda = \frac{\ln\left\{\frac{\left(\frac{1}{12}\left[E_{iv}^{f}+11F(\rho_0)+U_0\right]\right)}{AE_0\left[\ln\left(\frac{11}{12}\right)^{\alpha}-k\right]}\right\}}{\ln\left(^{11}/_{12}\right)} \quad (6)$$

With E_{iv}^{f} in equation (5) treated as a known physical input parameter. U_0 as the total energy per atom (negative of the cohesive energy E_0).

With the functions for GEAM and EAM obtained, the pair potential curves for the different models of Sr and Ir are plotted and compared with the universal pair potential curve of Rose et al. (1984).

RESULTS AND DISCUSSION

With the GEAM parameter $A = \pm 1$ and $\boldsymbol{\lambda}$ calculated from equation (6) using iterated values of α and K as in our preceding paper (Surface Energy calculation for fcc Metals with nagetive Cauchy's Discrepancy using the GEAM) and Oni-Ojo (2011). The fitting parameters and EAM functions are obtained and their values presented in Table 2 and Table 3, while the physical input parameters for Sr and Ir are in Table 1.

Table 1: Input Parameters for fcc metals Sr and Ir

	Lattice Constant a (Å)	Mono-vacancy Formation energy E_{iv}^{f} (eV)	Cohesion energy E_0 (eV)	Elastic constant (Gpa)			Bulk Modulus B (GPa)
				C_{11}	C_{12}	C_{44}	
Sr	6.0860	1.0800	1.7200	0.1532	0.0600	0.1002	0.1150
Ir	3.8400	1.9700	6.9300	5.9000	2.4900	2.6200	3.5500

Table 2: Calculated model's parameters for Sr corresponding to iterated values of α and K

EAM Parameter	Model				
	I	II	III	IV	V
A	-1.0000	-1.0000	-1.0000	-1.0000	-1.0000
α	0.9000	0.9200	1.0000	1.0500	0.9200
K	0.1500	0.2000	0.1000	0.1000	0.1500
λ	8.7648	6.9985	12.9397	13.2040	8.8520
V_{11} $[\rho_0]$ (-)	-0.4197	-0.4805	-0.2953	-0.2790	-0.4079
β	1.2590	1.4415	0.8858	0.8369	1.2237
P	4.5537	4.6401	4.3532	4.3130	4.5267
B_1	-2.2482	-2.2915	-2.2428	-2.2564	-2.2564
B_2	3.8807	3,9924	3.7798	3.7829	3.8811

Table 3: Calculated model's parameters for Ir corresponding to iterated values of α and K

EAM Parameter	Model					
	I	II	III	IV	V	VI
A	-1.0000	-1.0000	-1.0000	-1.0000	-1.0000	-1.0000
α	0.4800	0.5000	0.8800	0.9200	0.9400	0.9800
K	-0.3000	-0.3000	0.2000	0.2000	0.2000	0.1500
λ	-2.9789	-3.0566	9.2481	9.3918	9.4630	12.7096
V_{11} $[\rho_0]$ (-)	-0.8758	-1.0076	-1.0851	-0.5265	-0.4460	-0.3211
β	2.6275	3.0230	3.2554	1.5794	1.3380	0.9634
P	8.6432	8.9691	8.7367	6.7696	6.5008	6.2300
B_1	-5.0959	-4.9855	-7.6480	-8.6759	-8.8815	-8.8446
B_2	16.3264	16.7284	24.1933	20.7750	20.4908	19.7049

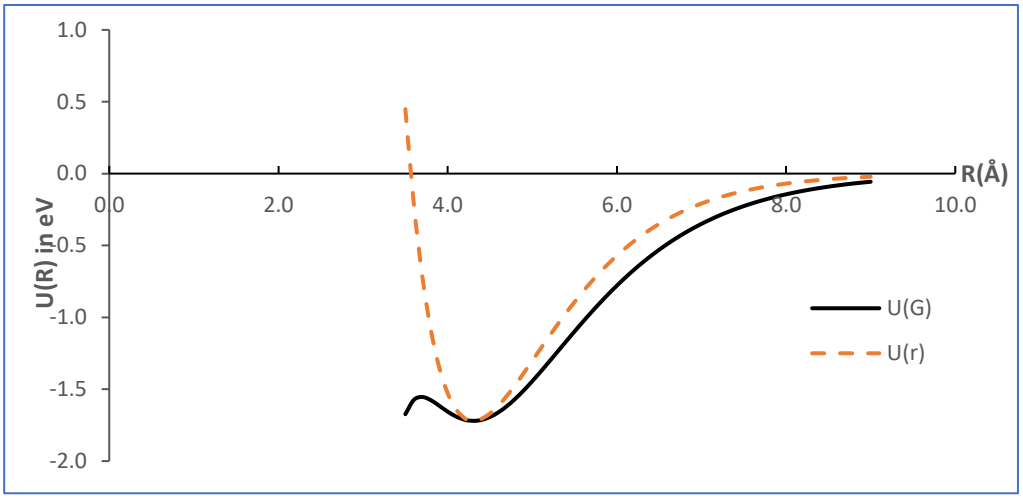

Figure 1: Potential curve for Sr Mod I

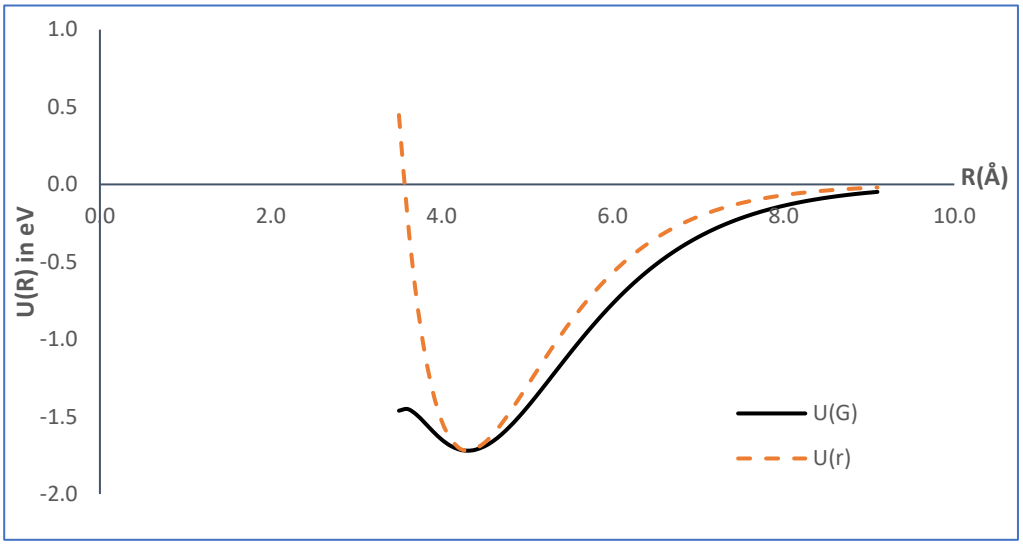

Figure 2: Potential curve for Sr Mod II

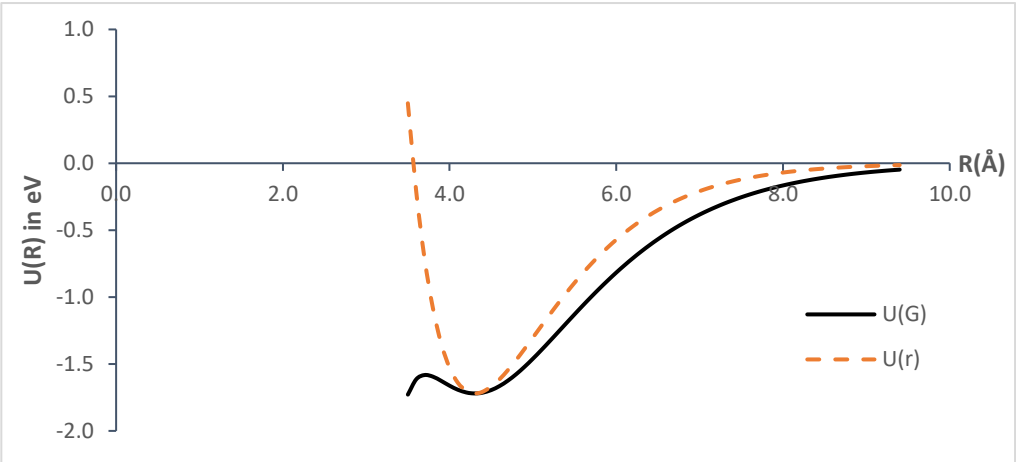

Figure 3: Potential curve for Sr Mod III

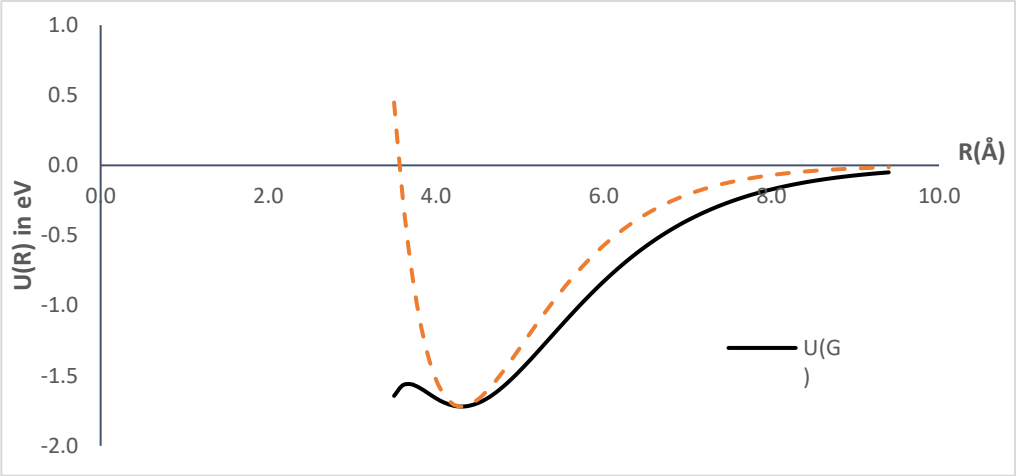

Figure 4: Potential curve for Sr Mod IV

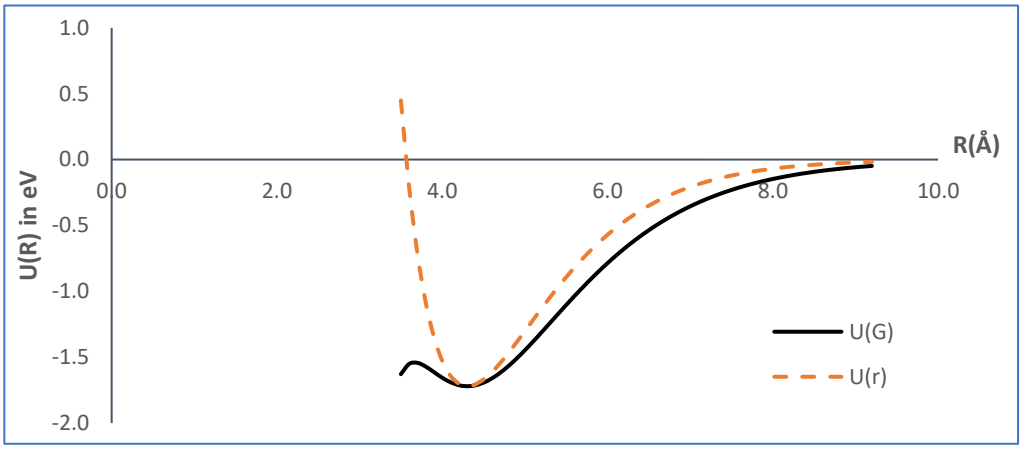

Figure 5: Potential curve for Sr Mod V

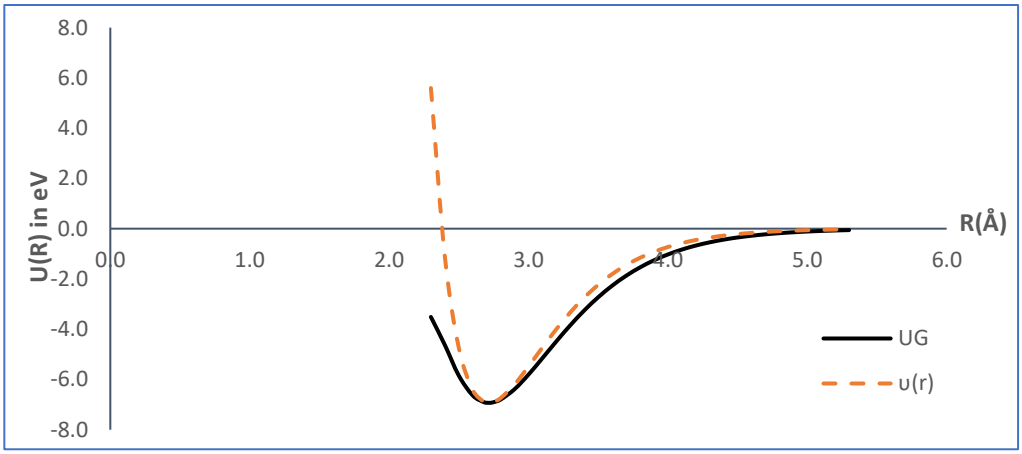

Figure 6: Potential curve for Ir Mod. IV

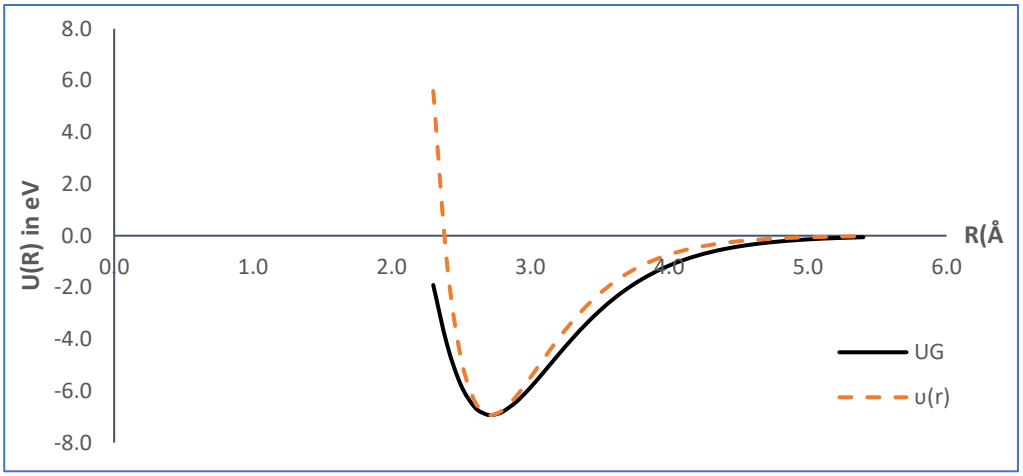

Figure 7: Potential curve for Ir Mod. V

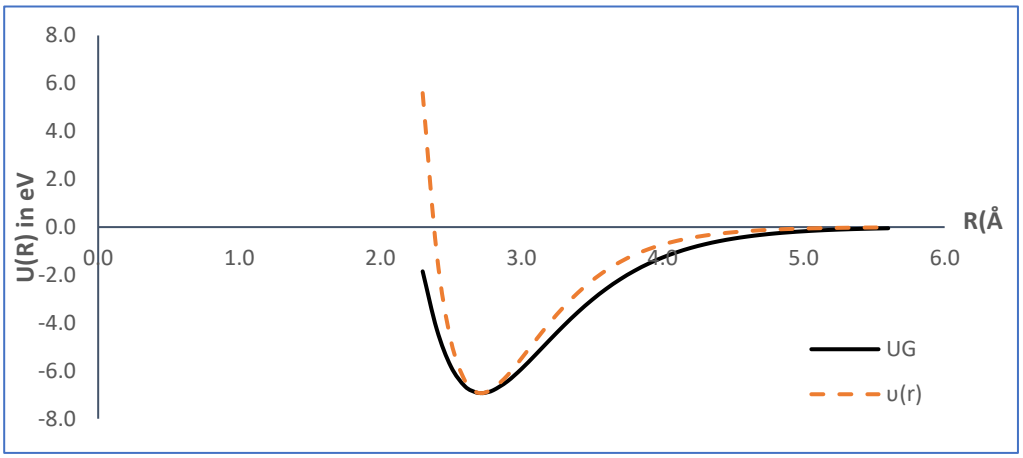

Figure 8: Potential curve for Ir Mod. VI

The fig.1 to fig.8 are for the inter-atomic potential curves predicted for Sr and Ir using GEAM iterated values in table 2 and Table 3. The thick lines are the GEAM pair potential curves while the dotted lines are the universal potential curves of Rose et al. (1984). Figures 1-5 are for the five selected Sr models but they do not show significant agreement with the Rose et al. (1984) curves, an indication that the iterated GEAM values selected may need to be further tested. The figures 6, 7 and 8 are for mod. 4, mod,5 and mod. 6 of Ir respective and their agreement with Rose et al. (1984) is good.

CONCLUSION

The inter-atomic potential curves above for Sr and Ir, using the GEAM have some of its models producing good results with the universal pair potential curves as in the case with Ir. The results obtained here are indications that the iterated values whose model matches could be a good result for fitting the GEAM parameters.

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