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GEAM investigation of the inter-atomic potential structure of Rhodium (Rh) as *fcc* metal having elastic constant with both $(C_{12} > C_{44})$ and $(C_{12} > C_{44})$

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ABSTRACT

The generalized embedding atom method GEAM, a model of the EAM designed by [1] was applied to study the surface energy status of Rh as fcc metal having both positive and negative Cauchy's discrepancy in our preceding papers. To further test the effectiveness of the model's parameters flexibility, this work has investigated the behaviour of the lattices of Rh by comparing the inter-atomic pair potential of both status Rh with that of [2] using the values predicted in our preceding work.

INTRODUCTION

Within the embedded - atom method (EAM) introduced by [3,4], which has been very effective in solving several properties of different metals such as: face-centred cubic (fcc), body-centred cubic (bcc), and diamond structures [4,5-10], are the works of other researchers that tried improving on the original EAM and had in turn introduced new models: the modified embedded-atom method (MEAM) [6,7], the analytical embedded atom method (AEAM) [10-13], the modified analytical embedded atom method (MAEAM) [14,15] and the Generalized embedded atom method (GEAM) [1].
Available records show that, besides predicting surface energies that are either too low or too high for fcc metals, most of the EAM models are unable to account for properties of metals with negative Cauchy discrepancy $(C_{12} < C_{44})$ [6, 16]. With the GEAM's iterated parameters values, good average surface energies results have been recorded for many fcc and bcc metals [16-20].
The focus of this study is to use the GEAM iterated values for Rh in our preceding paper and [20] to investigate the interatomic potential curve of Rh, using the input parameters given by two different

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researchers: In one, Rh was presented as fcc metal with positive Cauchy discrepancy $(C_{12} > C_{44})$[14] and in the second, the experimental value for C_{12} and C_{44} (at 300K) indicates $(C_{12} < C_{44})$ for Rh [22].That's, presenting Rh as a metal with negative Cauchy's discrepancy. The predicted pair potential curves in this work will be compared with the universal pair potential function curve of Rose et al to see how they match.

MATERIALS AND METHODS

In the GEAM, we have modified the embedding function of [21] to produce a four parameters generalized embedding function $F(\varrho)$.

$$F(\varrho) = AE_0(\varrho/\varrho_0)^{\lambda}\,[\ln(\varrho/\varrho_0)^{\alpha} - k] \quad (1)$$

Where, $\boldsymbol{A}$, $\boldsymbol{\lambda}$, $\boldsymbol{\alpha}$ and $\boldsymbol{K}$ are the GEAM parameters that provide flexibility to the model. Like every other models of the EAM, the total energy of a system in the GEAM, E_C is approximated to be, the sum total of the embedding and the pair potential function.

$$E_C = \sum_{j\neq i} F_i(\varrho_{h,i}) + \frac{1}{2}\sum \phi_{i,j}(R_{i,j}) \quad (2)$$

where $F(\varrho)$ denotes the embedding function, that is, the energy required to immerse an atom in the background electron density $\varrho(R)$ 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 $\boldsymbol{F_i(\varrho_{h,i})}$ 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 $\varrho(R)$, this work adopted a simple density function of the form that can be seen in other EAM,

$$\varrho(R) = \varrho_e \,.\, e^{-\beta.(\frac{r}{r_0} - 1)} \quad (3)$$

β is a parameter needed to fit the density function $\varrho(R)$.

For the pair potential, a 3-parameter model is adopted, which for large R is dominated by Johnson and Oh's exponentially decreasing function [13] given as,

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

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 ,

$$E_{iv}^f = 12F\left(\frac{11}{12}\varrho_0\right) - 11F(\varrho_0) - U_0 \quad (5)$$

gives

$$\lambda = \frac{\ln\left\{\dfrac{\frac{1}{12}[E_{iv}^f + 11F(\varrho_0) + U_0]}{AE_0[\ln(\frac{11}{12})^{\alpha} - k]}\right\}}{\ln(11/12)} \quad (6)$$

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 all the functions, GEAM and EAM obtained, the total energy curves for the thirteen Rh is plotted and compared with the Potential function of [2]

RESULTS AND DISCUSSIONS

The GEAM parameters are determined by fixing the parameter $A = \pm 1$, the parameter $\boldsymbol{\lambda}$ is obtained from equation (6) using iterated values of α and K as in our preceding paper and [20]. the fitting parameters and EAM functions are obtained and their values presented in Table 2 and Table 3, while the physical input parameters for Rh are in Table 1. Rh with $C_{12} > C_{44}$ is denoted with Rh(+) while that with $C_{12} > C_{44}$ is denoted as Rh(-).

Table 1: Input Parameters for fcc metals Rh(+)[14] and Rh(-)[22].

	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}	
Rh(+)	3.8034	1.7100	5.7500	4.1300	1.9400	1.8400	2.7000
Rh(-)	3.8034	1.7100	5.7500	4.1300	1.9200	1.9400	2.7000

Table 2: Calculated model's parameters for *Rh(+)* 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
$\boldsymbol{\alpha}$	1.8000	1.6500	1.6000	1.5000	0.4400
K	0.9000	0.7000	0.6500	0.5500	-0.1500
$\boldsymbol{\lambda}$	2.0558	2.1405	2.1531	2.1845	3.9897
V_{11} [ϱ_0] (-)	-0.2023	-0.2007	-0.2015	-0.2028	-0.1753
β	-0.6100	0.6000	0.6000	-0.6100	0.5300
P	-16.7100	10.1100	9.4700	8.4700	5.6000
$\mathbf{B_1}$	-0.7300	-2.0900	-2.4200	-3.0900	-7.6200
$\mathbf{B_2}$	8.3700	8.6700	9.0500	9.8500	15.5100

Table 3: Calculated model's parameters for *Rh(-)* 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
$\boldsymbol{\alpha}$	0.4400	1.6800	1.6800	1.6800	1.6400
K	-0.2500	0.1800	0.1400	0.1600	0.1600
$\boldsymbol{\lambda}$	-3.5253	12.8693	16.2189	14.3144	14.1830
$\mathbf{V_{11}}$ **[$\boldsymbol{\varrho_0}$] (-)**	-0.2588	-0.0461	-0.0404	-0.0433	-0.0447
β	0.7800	0.1400	0.1200	0.1300	0.1300
P	6.8100	5.1000	5.1700	5.1300	5.1400
$\mathbf{B_1}$	-5.0500	-8.3300	-8.0700	-8.2000	8.2000
$\mathbf{B_2}$	12.4400	15.8500	15.5200	15.6800	15.6800

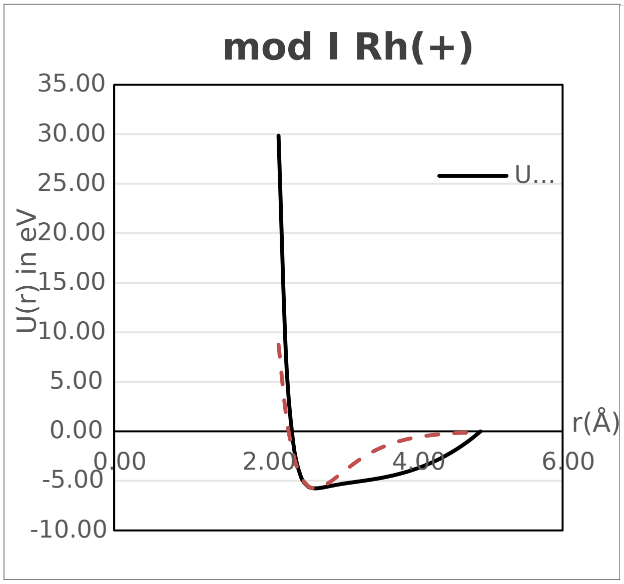

Fig. 1. Mod I Potential curve for Rh with $C_{12}>C_{44}$

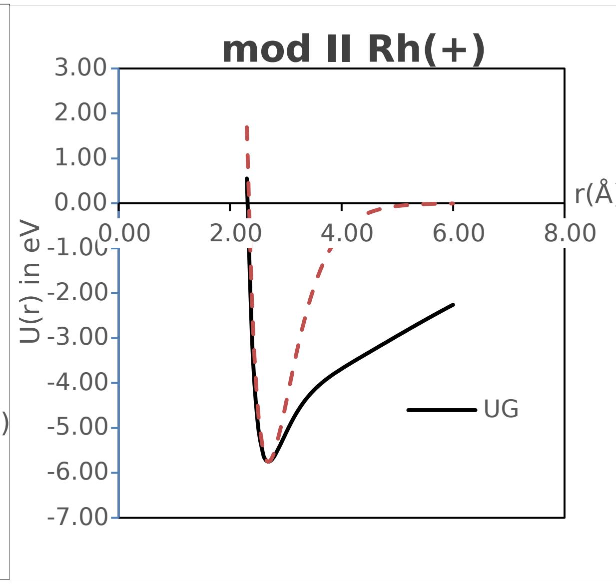

Fig. 2. Mod II Potential curve for Rh with $C_{12}>C_{44}$

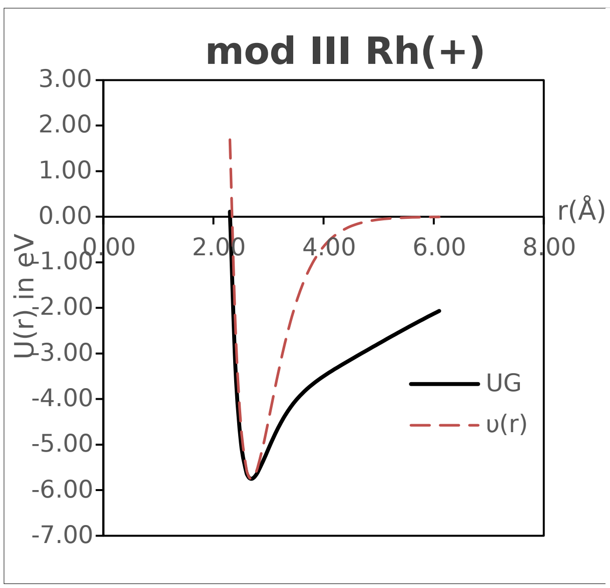

Fig. 3. Mod III Potential curve for Rh with $C_{12}>C_{44}$

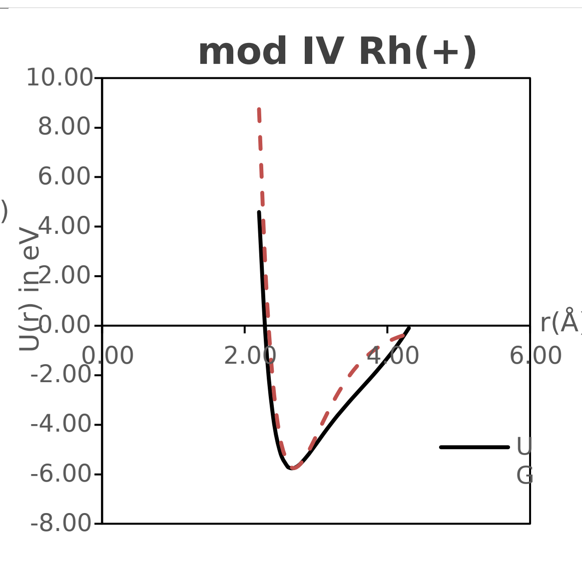

Fig. 4. Mod IV Potential curve for Rh with $C_{12}>C_{44}$

Fig. 5. Mod V Potential curve for Rh with $C_{12}>C_{44}$

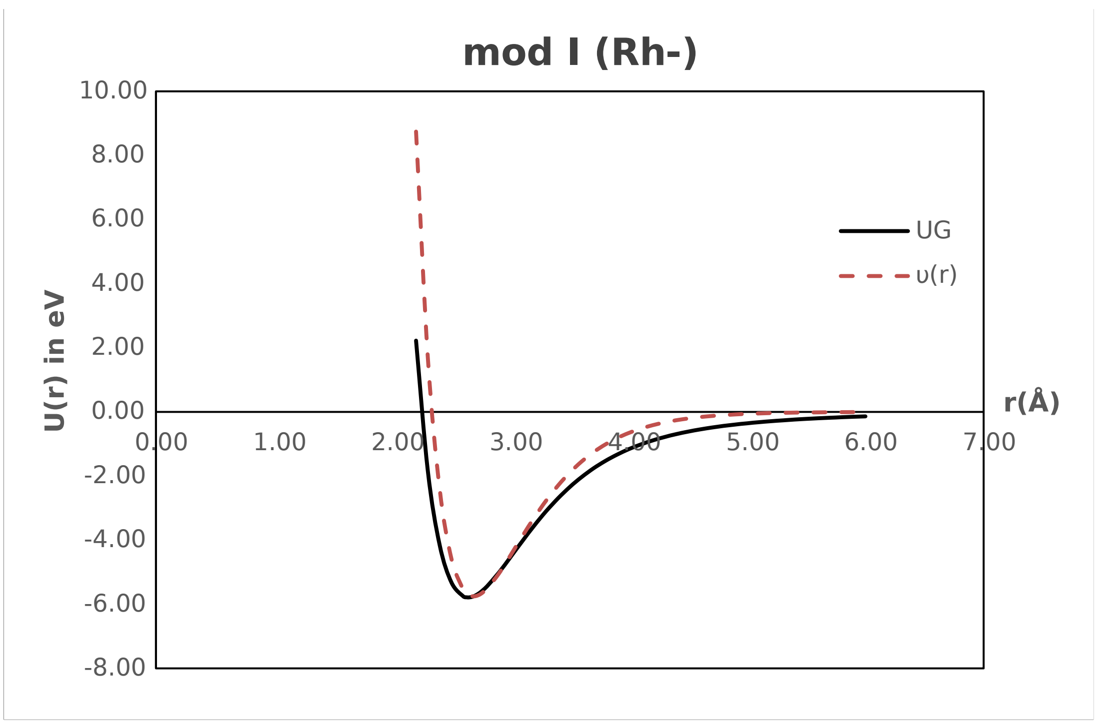

Fig. 6. Mod I Potential curve for Rh with $C_{12}<C_{44}$

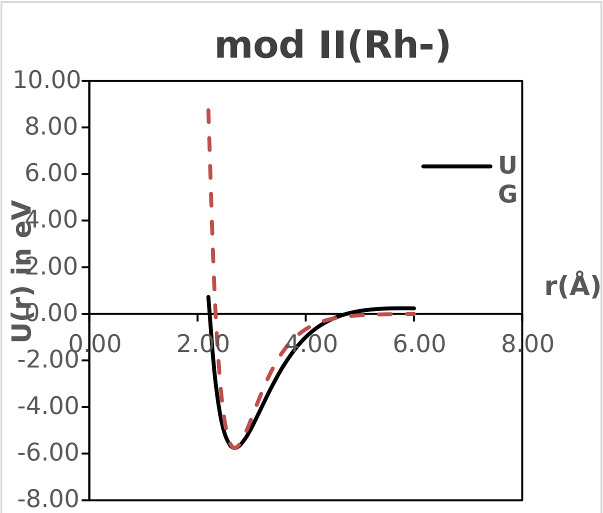

Fig. 7. Mod II Potential curve for Rh with $C_{12}<C_{44}$

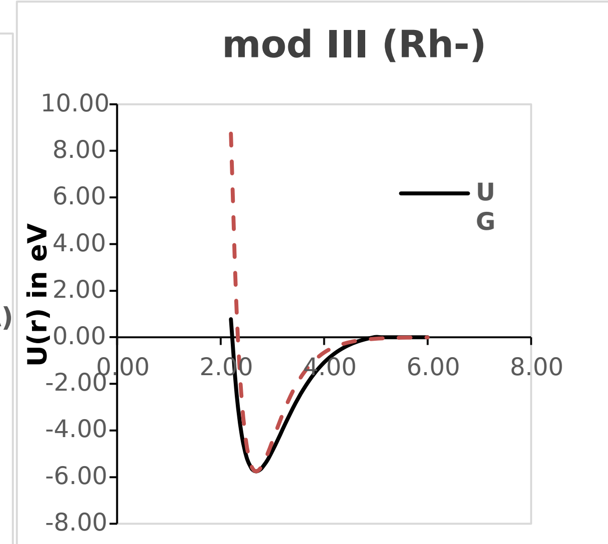

Fig. 8. Mod III Potential curve for Rh with $C_{12}<C_{44}$

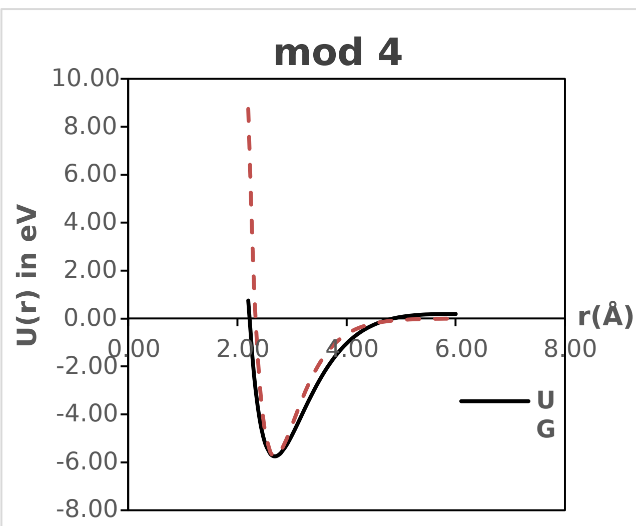

Fig. 9. Mod IV Potential curve for Rh with $C_{12}<C_{44}$

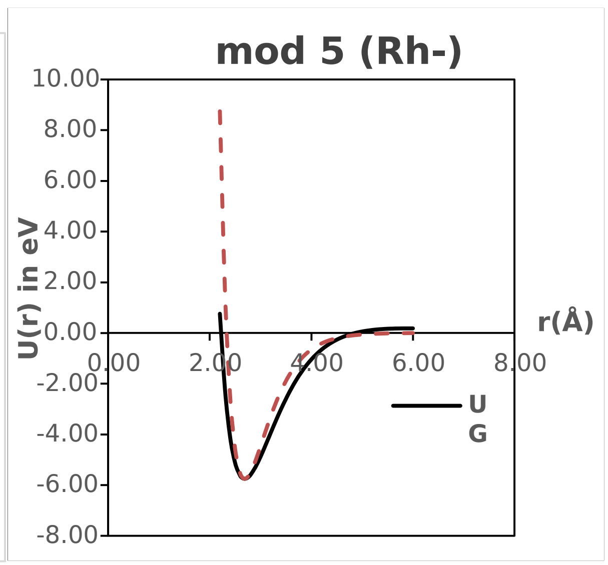

Fig. 10. Mod V Potential curve for Rh with $C_{12}<C_{44}$

Above are the curves of inter-atomic potential for Rh. The thick lines are for GEAM while the dotted lines are for universal curves of Rose et al. Figure 1-5 are for the GEAM iterated values for Rh with $C_{12} > C_{44}$. There is no match in the figures 1-4. Figures 6-10 are for Rh with $C_{12} < C_{44}$. Though there seems to be a match in the five of them, but the figure 6 and figure 5 both have a match that is a good agreement with the curve prescribed by the universal function of [2].

CONCLUSION

The inter-atomic potential curves above for Rh, using the GEAM have some of its models producing good results with the universal Rose et al.curves. 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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