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Surface Energy Calculation for some *transition* Metal Using the GEAM

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ABSTRACT
The three low index surface energies of fcc metals Cu, Ag, and Au are here calculated using the generalized embedded-atom method (GEAM). The low-index surface energies $\{\Gamma_{(111)}, \Gamma_{(100)}$ and $\Gamma_{(110)}\}$, with $\Gamma_{(111)}$ having the lowest and $\Gamma_{(110)}$ having the highest energy value. The anticipated values accord well with the experimental values.

INTRODUCTION

Surface energy is critical for understanding various surface phenomena such as absorption, corrosion, crystal formation, and so on.

The embedded - atom method (EAM) developed by Daw and Baskes (1983 and 1984) was used to determine surface energy for metals with face-centred cubic (fcc), body-centred cubic (bcc), and diamond structures (Adams and Foiles,1999, Baskes. 1992, Baskes and Nelson. 1989, Smith and Banerjia, 1987, Foiles et al, 1986, John, 1988 and Daw and Baskes, 1984). The EAM forecast for single crystal surface energy, on the other hand, is approximately 50% lower than the polycrystalline experimental value (Baskes, 1992).

The need to improve on Daws and Baskes' original work resulted in several modifications, including the modified embedded-atom method (MEAM) (Baskes, 1992, Baskes and Nelson, 1989) and Baskes, 1987), the analytical embedded atom method (AEAM) by Johnson et al. (1988, 1989 and 1990), and the modified analytical embedded atom method (MAEAM) by Zhang et al. (2008).

The surface energy of the *fcc* metals Cu, Ag, and Au is estimated in this study using the generalized embedded atom method (GEAM). The method and results are discussed below.

MATERIALS AND METHODS

Within the EAM, total energy of a system E_{tot} is approximated to be, the sum total of the embedding and the pair potential function.

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

where $F(\rho)$ denotes 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 $\boldsymbol{F_i(\rho_{h,i})}$ and $\phi_{i,j}$ and the parameters in each of these functions are determined by fitting to a limited set of bulk properties. If U_0 denotes the total energy per atom (negative of the cohesive energy E_0) and $\boldsymbol{\rho_{h,i}}$ is the electron density function at position R, then within a nearest neighbour model, it can be shown that for a monoatomic *fcc* solid (Daw and Baskes, 1984, Idiodi and Aghemenloh, 1998 and 1999 and Oni-Ojo et al. 2007).

$$U_0 = 6\phi_1(r_0) + F(\rho_0) \qquad (2)$$

$$0 = \phi_1'(r_0) + 3F'(\rho_0)\, V_{11}/r_0 \qquad (3)$$

$$\frac{3aB_0}{4} = \phi_1''(r_0) + \frac{a}{4\Omega_0}\{F'(\rho_0)[2W_{11} - 8W_{12} - 5V_{11}]\} - \frac{a}{4\Omega_0}\{2F''(\rho_0)V_{11}^2\} \qquad (4)$$

$$\frac{a}{4}C_{11} = G_{11} + \frac{a}{4\Omega_0}F'(\rho_0)W_{11} + \frac{a}{4\Omega_0}F''(\rho_0)V_{11}^2 \qquad (5)$$

$$\frac{a}{4}C_{12} = G_{12} + \frac{a}{4\Omega_0}F'(\rho_0)W_{12} + \frac{a}{4\Omega_0}F''(\rho_0)V_{11}^2 \qquad (6)$$

$$\frac{a}{4}C_{44} = G_{12} + \frac{a}{4\Omega_0}F'(\rho_0)W_{12} \qquad (7)$$

where $G_{11} = \frac{\phi_1'(r_0)}{2r_0} + \frac{\phi_1''(r_0)}{2}$ (8)

and $G_{12} = \frac{-5\phi_1'(r_0)}{4(r_0)} + \frac{\phi_1''(r_0)}{4}$ (9)

The equations (2) – (7), constitute the basic equations of the EAM and they depend on the fundamental functions $\boldsymbol{F(\rho)}$, $\boldsymbol{\rho(r)}$ and $\boldsymbol{\phi(r)}$.

The mono-vacancy formation energy E_{iv}^f is of the form;

$$E_{iv}^f = 12F\left(\frac{11}{12}\rho_0\right) - 11F(\rho_0) - U_0 \qquad (10)$$

E_{iv}^f is treated as a known physical input in this work. We derive (2.7) and (2.6).

$$\boldsymbol{V_{11}} = \pm\sqrt{\frac{\boldsymbol{\Omega_0(C_{12}-C_{44})}}{\boldsymbol{F''(\rho_0)}}} \qquad (11)$$

For metals with $C_{12} > C_{44}$, we demand that $F''(\rho_0)$ be positive definite while for metal with $C_{12} < C_{44}$, $F''(\rho_0)$ must be negative definite (Oni-Ojo et al. (2007).

RESULTS AND DISCUSSIONS

In a previous study, Oni-Ojo et al. (2007) modified the work of Yuan et al. (2003) to create a robust and flexible embedding function, which they called a generalized embedding function *F(ρ)*.

$$F(\rho) = AE_0\left(\rho/\rho_0\right)^{\lambda}\left[\ln\left(\rho/\rho_0\right)^{\alpha} - k\right] \quad (12)$$

Where λ, α and K consist in providing the flexibility. From 3.1, we obtain the three EAM parameters

$$F(\rho_0) = -AE_0k \quad (13)$$

$$F'(\rho_0) = \frac{-F(\rho_0)}{\rho_0}\left[\lambda - \frac{\alpha}{k}\right] \quad (14)$$

$$F''(\rho_0) = \frac{F(\rho_0)}{{\rho_0}^2}\left[\lambda^2 - \frac{2\lambda\alpha}{k} + \frac{\alpha}{k} - \lambda\right] \quad (15)$$

Where the differentiation with respect to the electron density, ρ, is indicated by the prime in equations (3.3) and (3.4). In this work, we achieved findings for A=+1 and A=-1 and the parameter, λ, α and K are chosen by requiring that the embedding function $F(\rho)$ fulfil equation (2.10) and thus,

$$\lambda = \frac{\ln\left\{\frac{\frac{1}{12}\left[E_{iv}^{f} + 11F(\rho_0) + U_0\right]}{AE_0\left[\ln\left(\frac{11}{12}\right)^{\alpha} - k\right]}\right\}}{\ln\left({}^{11}/_{12}\right)} \quad (16)$$

After determining, λ from 3-5, using the iterated values for α and **K**, the EAM functions and parameters are determined. Using the input parameters in Table 1, the calculated displayed in Table 2, Table 3 and Table 4.

Tables 5-7 shows the Surface energy of three low-index surfaces for the examined fcc metals for the various GEAM iterated values for A, α and **K** (Oni-Ojo, 2011).

Table 1: Table of Physical input Parameters: ***Lattice Constant a (Å), Bulk Modulus (GPa) Elastic Constant (GPA), Cohesive and mono-vacancy formation energy (eV)***

	Cohesion energy E_0 (eV)	Mono-vacancy Formation energy E_{iv}^{f} (eV)	Lattice Constant *a* (Å)	Elastic constant (Gpa)			Bulk Modulus *B* (GPa)
				C_{11}	C_{12}	C_{44}	
Cu	3.54	1.30	3.16	1.68	1.21	0.750	1.37
Ag	2.85	1.21	4.09	1.24	0.93	0.460	1.01
Au	3.93	0.89	4.08	1.89	1.59	0.420	1.73

Table 2: EAM Model Parameters for fcc Cu calculated from iterated GEAM values of α and K.

Parameters	Model					
	I	II	III	IV	V	VI
A	-1	-1	-1	-1	1	1
α	0.0100	0.0300	0.0600	0.1400	0.4600	0.9000
K	0.2000	0.3000	0.2000	0.2500	-0.1500	0.1000
λ	4.9476	3.5462	5.1939	4.5520	2.9918	2.4245
$F(\rho_0)$ [eV]	0.7080	1.0620	0.7080	0.8850	0.5310	-0.3540
$F'(\rho_0)$[eV/ρ_0]	3.4675	3.6598	3.4649	3.5330	3.2170	2.3277
$F''(\rho_0)$[eV/$\rho_0$2]	13.5133	8.9419	13.4280	10.2932	11.2793	11.0401
V_{11} [ρ_0] (-)	-0.4999	-0.6145	-0.5015	-0.5728	-0.5472	-0.5531
W_{11} [ρ_0]	-2.9633	-3.0894	-2.9680	-3.0727	-3.2108	-4.0311
W_{12} [ρ_0]	-0.4354	-0.3421	-0.4352	-0.3863	-0.4652	-0.7445
$\phi_1(r_0)$ [eV]	-0.7080	-0.7670	-0.7080	-0.7375	-0.6785	-0.5310
$\phi_1'(r_0)$[eV/Å]	0.3396	0.4406	0.3404	0.3965	0.3449	0.2522
$\phi_1''(r_0)$[eV/Å^2]	2.8184	2.9371	2.8193	2.8852	2.8245	2.7157

Table 3: EAM Model Parameters for fcc Ag calculated from iterated GEAM values of α and K

Parameters	Model					
	I	II	III	IV	V	VI
A	1	-1	1	-1	1	1
α	0.85	0.01	0.04	0.06	2	1.35
K	0.08	0.20	-0.20	0.20	1.75	0.60
λ	2.7414	4.5347	4.2831	4.7810	1.7510	2.0941
$F(\rho_0)$ [eV]	-0.2280	0.5700	0.5700	0.5700	-4.9875	-1.7100
$F'(\rho_0)$[eV/ρ_0]	1.7975	2.5563	2.5553	2.5542	-3.0332	0.2666
$F''(\rho_0)$[eV/$\rho_0$2]	9.7712	8.9065	8.8776	8.8397	7.7028	8.3488

V_{11} $[\rho_0]$ (-)	-0.7166	-0.7506	-0.7518	-0.7534	-0.8071	-0.7752
W_{11} $[\rho_0]$	-5.9322	-4.6647	-4.6683	-4.6730	1.0519	-31.8886
W_{12} $[\rho_0]$	-1.4458	-0.8932	-0.8931	-0.8929	1.4726	-11.7777
$\boldsymbol{\phi_1(r_0)}$ [eV]	-0.4370	-0.5700	-0.5700	-0.5700	0.35625	-0.1900
$\phi_1'(r_0)$[eV/Å]	0.2227	0.3317	0.3321	0.3327	-0.4233	0.0357
$\boldsymbol{\phi_1''(r_0)}$[eV/Å^2]	2.1807	2.2938	2.2942	2.2948	1.5106	1.9867

Table 4: EAM Model Parameters for *fcc* Au calculated from iterated GEAM values of α and K

Parameters	**Model**				
	I	**II**	**III**	**IV**	**V**
A	-1	-1	1	1	1
$\boldsymbol{\alpha}$	0.06	0.62	1.05	1.9	0.95
K	0.2	0.2	0.05	0.9	0.08
$\boldsymbol{\lambda}$	6.2755	8.7239	2.8521	2.0735	1.9067
$F(\rho_0)$ [eV]	0.7860	0.7860	-0.1965	-3.5370	-0.3144
$F'(\rho_0)$[eV/ρ_0]	4.6967	4.4204	3.5661	0.1331	3.1340
$F''(\rho_0)$[eV/$\rho_0$2]	23.2978	12.8860	18.3741	15.6255	9.9601
V_{11} $[\rho_0]$ (-)	-0.7295	-0.9809	-0.8215	-0.8908	-1.1157
W_{11} $[\rho_0]$	-5.1651	-5.8996	-6.5241	-132.5401	-7.7855
W_{12} $[\rho_0]$	-1.3529	-1.3346	-1.8515	-60.1573	-2.0163
$\boldsymbol{\phi_1(r_0)}$ [eV]	-0.786	-0.7860	-0.6223	-0.0655	-0.6026
$\phi_1'(r_0)$[eV/Å]	0.5938	0.7515	0.5077	0.0206	0.6060
$\boldsymbol{\phi_1''(r_0)}$[eV/Å^2]	3.6256	3.7895	3.5360	3.0294	3.6383

Table 5: The table below shows the projected low-index surface energy for Cu in Ergs/cm^2 and the average experimental value for Cu (Aghemenloh and Idiodi, 1998)

Model	**Present work**				**EXPERIMENT**
	Γ_{111}	Γ_{100}	Γ_{110}	**AVERAGE**	
I	1492.0011	1974.0662	2116.5025	1860.856573	1830.00
II	1365.7000	1800.5262	1957.8670	1708.031039	
III	1490.8541	1972.8475	2115.6794	1859.793654	
IV	1411.6613	1866.9779	2021.6806	1766.773263	
V	1452.8760	1930.9304	2088.0868	1823.964406	
VI	1466.3795	1961.8421	2130.9221	1853.0479	

Table 6: The table below shows the projected low-index surface energy for Ag in Ergs/cm^2 and the average experimental value for Ag (Aghemenloh and Idiodi, 1998)

Model	**Present work**				**EXPERIMENT**
	Γ_{111}	Γ_{100}	Γ_{110}	**AVERAGE**	
I	1024.4819	1348.1132	1451.1536	1274.5829	1250
II	977.3479	1269.0229	1363.4810	1203.2839	
III	976.9512	1268.5620	1363.1366	1202.8833	
IV	976.5354	1268.1166	1362.8343	1202.4954	
V	991.9638	1315.1883	1437.4634	1248.2052	
VI	1001.6413	1323.7845	1438.4398	1254.6219	

Table 7: The table below shows the projected low-index surface energy for Au in Ergs/cm^2 and the average experimental value for Au (Aghemenloh and Idiodi, 1998)

Model	**Present work**				**EXPERIMENT**
	Γ_{111}	Γ_{100}	Γ_{110}	**AVERAGE**	
I	1186.6116	1647.6869	1749.4613	1527.9199	1500.00
II	1143.2138	1613.7648	1733.1691	1496.7159	
III	1158.5969	1643.0255	1779.1010	1526.9078	
IV	1121.8042	1610.7277	1773.4017	1501.9779	
V	925.5485	1301.8759	1447.4374	1224.9540	

The average values of the Surface energies for the three metals as presented in the tables 5-7 show a range of deviations from experimental values: For Cu is between 1.6% to 6.7%, For Ag is between 1.9% to 3.8% and for Ag is 1.8% to 18.4%.

CONCLUSION

The three low-index surface energies of Cu, Ag, and Au were computed using GEAM iterated parameter values, and the findings show a general trend of $\Gamma_{111} < \Gamma_{100} < \Gamma_{110}$ for all values, with their average being in good agreement with the experimental average. As a result, the GEAM will be a useful instrument for calculating relative values of surface energy and other metal properties. A method for characterizing and fitting the GEAM parameters, $\boldsymbol{\alpha}$ and K, using appropriate equations is being investigated.

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