CALCULATION OF SURFACE RELAXATION OF Fe, W AND Mo METALS USING ANALYTICAL EQUIVALENT CRYSTAL THEORY

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CERTIFICATION

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DEDICATION

This project is dedicated to God Almighty for his continuous strength and grace to see me through this phase of life and to my family most especially Mrs. Vivian Okpako and Mrs. Jennifer Itulua and my fiance Josephine for their perennial and noble/ethical financial support.

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TABLE OF CONTENT

ABSTRACT

I have used the newly formulated Analytical Equivalent Crystal Theory method which is a modification of the AECT method is use to calculate the surface energies and surface relaxation for three low-index surface of Bcc transition metals. Fe,W and Mo.

Our calculations predicted top layer contractions for the Bcc metals in reasonable agreement with experiment and theory. The data may be used as a starting point for models of surface science phenomena.

The accuracy of the surface energies and relaxation is established from a comparison with other theoretical results and experiments.

CHAPTER ONE

1.1. INTRODUCTION

Relaxation and reconstruction processes at metal surface have attracted the interest of the scientific community for decades. The reason is that knowledge of the geometrical arrangement of the atoms in the vicinity of the surface is a basic ingredient for any study of structural and dynamical properties of a metal surface. It is well known that real surfaces of pure metals can adopt different structures from those of ideally truncated crystal. During relaxation only the rigid inward or outward displacement of the atomic layers occurs, while in case of reconstruction, the displacement of atoms may alter the two-dimensional symmetry of the surface. Experimental studies have demonstrated that the surface layer of most clean transition metal surfaces relaxes inward [1], that is, the inter-layer distance between the topmost two atomic layers is smaller than in the bulk. Expansion of the top layer has also been found for some surfaces of noble metals. The top layer relaxation is often accompanied by relaxation of the surface atomic layers, resulting in an oscillatory multi-layer relaxation.

Several theoretical models have been proposed to explain the surface relaxation of transition metals [2]. Extensive experimental investigation with the low energy electron diffraction (LEED) [3-11], low and medium energy ion scattering (LEIS, MEIS) [12,13], and by other techniques [14,15], have been done on FCC metals. Several semi-empirical calculations, such as equivalent crystal theory method (ECT) [16], embedded atom method (EAM) [17,18], modified embedded atom method (MEAM) [19-20], effective medium theory (EMT) [21], and

tight-binding potential (TB) [22], has also been done on FCC metals. Some density functional theory (DFT) [23-32] and related [33] calculations exist as well. However, this is not the case with Bcc metals. To our knowledge, surface relaxation calculations for Bcc metals are scarce, in that only few results are available in the literature.

Surface energy and surface relaxation of Fcc and two Bcc materials [16, 34,35] have been calculated using the original equivalent crystal method (ECT) developed by smith and co-workers [34,35]. Recently, an extension of the ECT was introduced by Zypman and Ferrante [36]. The analytical equivalent crystal theory method (AECT) which has been shown to increase the computational speed of the ECT has also been extensively used to describe the energetic of defects in metals [37, 38]. However, it has not been applied to calculate surface relaxation in Fcc and Bcc metals. The purpose of this present work is to apply the AECT in calculating surface relaxation and surface energy of a large number of Bcc metals for the three low index Surface.

1.2. The Aim of this study is to:

Calculate the surface relaxation energy of the Bcc metals Fe,W and Mo using the Analytical Equivalent Crystal Theory (AECT)

1.3. The Objective of this study is to:

Obtain the surface relaxation of Fe,W and Mo metals.

And to compare the results obtained with the previous theoretical work in the literature and experiment.

This project is structured as follows. In chapter two, we give a brief discussion of the Analytical Equivalent Crystal Theory (AECT). In chapter three, we discuss the AECT method of calculating the surface relaxation and surface energies of Bcc metals. The results of surface energies and relaxation for 3 Bcc metals are reported in chapter four, along with the results obtained, chapter five summarizes the findings, conclusion and suggestion for further studies.

CHAPTER TWO

2.1. THE ANALYTICAL ECT METHOD

In ECT, the total energy of a collection of atoms near a defect is the sum of energy relation contributions U(a_{eq}) is explicitly given by the universal binding energy relation (UBER) which is simply parameterized in terms of physical known constants in the Rydberg function. In ECT an atom near a defect is viewed as sensing a reduce or increased electron density. This conditions is then interpreted as a point on the IJBER in terms of an expanded or contracted perfect crystal perturbation theory is used to obtain the equivalent lattice parameter of the expanded or contracted crystal, a_{eq} in terms of the lattice parameter corresponding to the perfect crystal. Once a_{eq} the lattice parameter corresponding to the perfect crystal once a_{eq} is known, the energy of the atom near the defect is obtained from that point on the UBER. The value leqis obtained in terms of a_o from the inversion of the basic ECT transcendental equation. Although conceptually simple, the inversion process represents the computational time limiting step in the implementation of the algorithm. The implementation of ECT involves a perturbation equation that determines the energy of a solid with a defect in terms of a perfect crystal of the same substance expanded or contracted from the parameter. This equilibrium lattice parameter to a new "equivalent" lattice parameter. This procedure is equivalent to finding an embedded electron density produced by the electronic charge density of the remainder atoms in the system. The yet unknown, equivalent nearest-neighbour distance, R_{eq} satisfies.

$N_1 R^{P}_{eq} e^{zReq} + N_2 (C_2 R_{eq})^{p} e^{-(x+1/4)} C_2 R_{eq} = p$

Where N_1 is the number of nearest-neighbour in the minimum energy crystal structure corresponding to that atom, N_2 is the number of next nearest neighbour, C_2 is the ratio of the next-nearest neighbour distance to the nearest-neighbour distance and and are known material-dependent constants. In many applications of ECT to evaluate defect formation energies, p on the right hand side of Eq.1, is written in a form similar to the left hand side. For example, the density produced by neighbour on an atom next to a vacancy is

$P = N^1_1 R^p_0 e^{-aRo} + N^1_2 (c_2 R_{eq})^p e^{-(a+1/)} C_2 R_0$

Where $N^1_1 = N_1 - 1$ and $N^2_1 - N_2$ because the atom in question loses one nearest-neighbour (where the vacancy is located) and no second near neighbour. In this example, the lattice is unrelaxed and consequently R_0 represents the nearest-neighbour distance of the perfect crystal. This shows explicitly that Re is the unknown in Eq.(1). once R_{eq} is obtained, ECT uses this value in the UBER function, $U(a_{eq}) - U(a_0)$ in what follows, we adopt the method of Zypman and Ferrante. The general problem is therefore to find the function.

$R_{eq} = G(p)$

Eq.(1) can be cast in dimensionless form by defining

$$y = aR_{eq}$$

$Y^p e^y + N_2/N_1 C^p_2 y^p_e (1 \text{ I } 1/a) C_2 -1 = y$, $N_2/N_1 = n_{21,}$ $pa^p/ N_1 = x$,

By introducing $(1 + n_{21} C^P_2 y^p e^{-Yy}) = x$

The constant (a) is about unity or larger and $C_2 > 1$, thus y > 0. which is a conservative lower bound for y. By using appropriate values from Table 1, one finds that $n_{21}\, C^{p}{}_{2} y^{p}\, e^{-Yy} < 0.25$ in the table 2. thus, in Eq. 4, the second term inside the parenthesis is much smaller than unity, and therefore it is dropped in many real applications. Thus, the problem reduces to finding the roots of

$$Y^{p}\, e^{-y} = x$$

A sketch of Eq.(5) is shown in fig. 1. The root y_1 correspond to the smaller lattice parameter while the root y_2 corresponds to the larger lattice parameter. Creating a vacancy effectively lowers the atom density thereby increasing y. thus the physically accepted root is y_2

Eq. (5) can be recast in the Lambert form:

$$(-y/p)\, e^{(-y/p)} = -x^{1/p}/p$$

With the solution

$$(-y/p)\, e^{(-y/p)} = -x^{1/p}/p$$

Where w_1 is the Lambert function [17,18]. the sub index ‘’-1” labels the branches. The Lambert function has an infinite number of complex branches with only two purely real, the branches known as ‘0’ and ‘-1’.

Define ($Y_m X_m$) as the point corresponding to the maximum attainable density. y_M may be found by taking the maximum of Eq. (4) as

$$P - ym + n_{21} C^{2}_{p}\, e^{-Yym} [\, P - (\, 1 + y\,) y_m\,] = 0$$

Again, taking the inverse of maxima of eq.(9) to obtain y, we have the only non-trivial solution to Eq.(10) is for the argument of the Zero

branch to be ---I/e. for a complete discussion of the above equation and the conditions that lead to its derivations, the interested reader is referred to the work of Zypman and Ferrante, the smallest possible value of (y) is given as

Eq.(11) was used to evaluate the y_{min}.

CHAPTER THREE

3.1. CALCULATION OF SURFACE ENERGY

Here, we implement the analytical algorithm of the ECT by Zypman and Ferrante. The surface energies of the three low-index planes of 3 BCC metals are obtained by this algorithm. However, it is emphasized that only the volume of the ECT is retained, while neglecting the other terms. The neglect of the higher order terms of the ECT justified from previous studies [10, 19, 20]. In what follows we first solve Eq. (4) numerically, and then by the Lambert function as given by [15].

For the real density of the (110) plane, we noticed that a typical surface atom has lost 2 nearest-neighbours (out of 8 in bulk) and 2 next nearest neighbors (out of 6 in bulk). Then

$$p = 6R^{P}_{0} \exp (- aR_0) + 4 (C_2R_0)^{P} \exp [\left(\sigma + \frac{1}{\Lambda}\right) C_2 R_0 - \quad - \quad (12)$$

Where $\sigma, \rho \; and \; \Lambda$, are material constant whose values depends on each *metal, and C_2 and R_0 are given as $R_2 = \frac{a\sqrt{3}}{2}$, $C_2 = \frac{2}{\sqrt{3}}$. Solving Eq. (12), we obtain the value of electron density p

Next we solve

$$X = \frac{\rho\sigma^{\rho}}{8} \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad (13)$$

And then using the product Log function in mathematics, we get

$$y = -p\, Productlog\,[-1, \frac{-X^{\frac{1}{p}}}{P}] \quad - \quad - \quad - \quad - \quad - \quad - \quad (14)$$

Now, after obtaining the value of y from Eq. (14) we then compute the nearest neighbour distance R_{eq} from the relation.

$$R_{eq} = \frac{Y}{\sigma} \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad -- \quad (15)$$

Once the value of y has been obtained from Eq. (14) and knowing the value of the material constant , we can then calculate the value of R_{eq} from Eq.(15). next we compute the lattice parameter a_{eq} from $a_{eq} = c_2 R_{eq}$

$$- \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad - \quad (16)$$

For the real density of the (100) plane of a BCC lattice, three surfaces are involved. An atom in the surface plane (j=1) and the first surface below the surface plane (j=2). The equation for p to be solved ar :

$$p = 4Rp0\ exp\ (-aR0) + 5\ (C_2R_0)P\ exp\left[-\left(\sigma+\frac{1}{\Lambda}\right)C_2R_0\right]-$$

$$-\ -$$

$$-\qquad\qquad 17a)$$

and

$$p = 8Rp0\ exp\ (-aR0) + 5\ (C_2R_0)P\ exp\ [-(a + 1/\ )\ C_2R_0]\ -$$

$$----------\ (17b)$$

But in the case of the (1 1 1) plane of a Bcc lattice, three surface are involved. An atom in the surface plane (j=1) has lost 4 nearest-neighbors and 3 next nearest-neighbor atom. An atom in the second plane (j=2) has lost 1 nearest-neighbor atom and 3 next nearest-neighbor atoms, while an atom in the third plane (j=3) has lost only 1 nearest - neighbour atom. Therefore, the equations to be solved are :

$$p = 4R\frac{p}{0}\ exp\ (-aR0) + 3\ (C_2R_0)P\ exp\ [-\left(\sigma+\frac{1}{\Lambda}\right)C_2R_0]\ --$$

$$----------\ (18a)$$

$$p = 7R\frac{p}{0}\ exp\ (-aR0) + 3\ (C_2R_0)P\ exp\ [-\left(\sigma+\frac{1}{\Lambda}\right)C_2R_0]\ -$$

$$----------\ (18b)$$

$$And$$

$$p = 7R\frac{p}{0}\ exp\ (-aR0) + 6\ (C_2R_0)P\ exp\ [-\left(\sigma+\frac{1}{\Lambda}\right)C_2R_0\ ]\ -$$

$$----------\ (18c)$$

Eqs. (17) and (18) are then solved for p and Eqs. (13) and (14) for x and y. thereafter, Eqs. (15) and (16) are solved for R_{eq} and a_{eq} for each Bcc metals.

Once the value of R_{eq} are known from Eqs. (15), then the values of a and F can be calculated directly [6]. the surface energy for each of the three low-index faces is then calculated from the formulas.

$$\sigma_{111} = \frac{\Delta}{a^2\sqrt{3}} \sum_j F\,[a1\,(j)] \qquad - - - - - - \qquad (19)$$

$$\sigma_{110} = \frac{\sqrt{2}}{a^2\sqrt{3}} \Delta E \sum_j F\,[a1\,(j)] \qquad - - - - - - \qquad (20)$$

$$\sigma_{100} = \frac{\Delta\,\mathrm{E}}{a^2} \Delta\mathrm{E}\ \sum_j F\,[a1\,(j)] \qquad - - - - - - \qquad (21)$$

The sum over j includes only one atom per atomic layer and usually only a few layers need to be included for metal low index planes.

Table 1: pure metal properties and the calculated ECT constants for Bcc metals. Lattice constants and cohesive energy E are from Ref. [ ], Bulk modules B are from Refs.[ ].vacancy formation energies E_{iv} are from Refs. [ ]

Element	E(eV)	A (A′)	E^{f}_{iv}(eV)	B($10^{11}$$jm^{-3}$)	P	L(A·)		a(A^{0-1})	V_{WSE}(A)
Mo	6.82	3.15	3.0	2.725	8	0.262	0.736	3.597	1.551
W	8.66	3.16	4.0	3.23	10	0271	0.760	4.243	1.556
Fe	4.29	2.86	1.6	1.68	6	0.278	0.780	3.110	1.408

Table 2 : Smallest value of y (=y_{min}) and the corresponding values for 3 Bcc metals.

Element	y_{min}	$Y=(1+1/a)c_{2-1}$	$Z=n_{21}C^{p}e^{-yy}$
Mo	7.481	0.591	0.029
W	9.377	0.513	0.026
Fe	5.573	0.631	0.053

CHAPTER FOUR

4.1. RESULT AND DISCUSSION

The equivalent crystal nearest neighbor distance R_{eq} is a very vital parameter in the ECT method, since it is the parameter needed in the calculation of surface energy. R_{eq} values are also needed in the computation of a_{eq}, the equivalent lattice parameters a_{eq} is shown in Table 2 which displays the relatives difference between the Lambert evaluation method (AECT) and the numerical evaluation (Newton - Raphson method) of the ECE. A comparison of the present work with a previous study [21] which used the old ECT is presented in the table 3. It can be seen from the table that there is a good agreement between the two ECT methods. R_{eq} has been employed to calculate the values of surface energies in table 4c compares well with an earlier result [21]. this is clearly seen in Fig 2.

The surface energies obtained for the three low-index faces of the Bcc metal are presented in table 5 for comparison, we also present some theoretical results and experimental derived values.

These theoretical methods include, first-principles calculated in ref [13-5, 22-25], the tight-binding (TB) method in Ref. [26], the jellium model in Ref. [27], the embedded atom method (EAM) in Ref.[28] the Modified Embedded Atom Method (MEAM) in Ref. [29], the Modified Analytical Embedded Atom Method (MAEAM) in Ref. [30], and experimental from Refs.[1,2]. The experimental values are determined from measurements of the surface tension of liquid metals, it can be seen that our AECT surface energy results are uniformly larger and closer to experiment and first-principles measurements of the surface energy are more commonly

found for poly-crystalline materials. Table 5 also shows that our calculated surface energy of each (h k 1) plane in alkali metals are much lower than that in transition metals in good agreement with FCD [5] and experiment [2] as shown in Fig 3. Fu et al. [23] have used density functional theory to calculate the (1 0 0) surface energy in the metals W and V. their calculated values for W and V of 5.1jm^2 and 3.4jm^2 respectively are in good agreement with the present values calculated using AECT.

Table 3: Rigid and relaxed surface energies (in jm^{-2}) for Bcc metals.

Element	Crystal Face(hkl)	Rigid	Relaxed		
Mo	(100)	4.877	4.776	4.741	0.035
	(110)	2.604	2.564	2.542	0.022
	(111)	3.505	3.384	3.341	0.043
W	(100)	5.904	5.835	5.806	0.029
	(110)	3.279	3.253	3.237	0.016
	(111)	4.319	4.212	4.165	0.047
Fe	(100)	3.474	3.379	3.349	0.030
	(110)	1.748	1.720	1.698	0.022
	(111)	2.442	2.331	2.288	0.043

Table 4: Experimental and theoretical surface energies (in jm^{-2}) for Bcc metals.

Element	Crystal face(hkl)	AECT (present)	Semi empirical calculations	First principles calculations	Expt.
Mo	(100)	4.776	2.120[a],2.286[b],2.122[c], 2.2332[d],3.130[e]	3.837[f], 3.520[j]	
	(110)	2.564	3.0404[a],2.127[b],1.930[c] 2.188[d], 2.885[e]	3.454[f] 3.180[g] 3.14[j]	3.000[l], 2.907[m]
	(111)	3.384	2.840[a], 1.861[c], 2.678[d], 3.373[e]	3.740[f].	
W	(100)	5.835	6.700[a],2.809[b], 2.646[c], 2.638[d] 3.900[e]	4.635[f] 5.100[h] 4.780i	
	(110)	3.253	4.300[a],2.599[b], 2.232[c], 2.638[d], 3.427[e]	4.005[f], 3.840[g]	3.680[l], 3.625[m]
	(111)	4.212	6.750[a], 2.247[c], 3.315[d], 4.341[e]	4.452[f]	
Fe	(100)	3.379	1.685,2.289[c], 1.537[d],2.510[e]	2.222[f]	
	(110)	1.720	6.700[a],1.135[b], 1.566[c],1.429[d],2.356[e]	2.430[f], 3.090[g]	2.480[l], 2.417[m]
	(111)	2.331	1.720[c] 1.772[d] 2.668[e]	2.733[f]	

Table 4 Reference (BCC)

a) Tight-Binding total energy calculations (TB), Ref.[24]
b) Embedded atom method calculations (EAM), Ref.[28]
c) Modified embedded atom method calculations (MEAM). Ref [29]
d) Modified analytical embedded atom method (MEAM), Ref.[30]
e) Modified embedded atom method (SNNMEAM), Ref.[23,24]
f) FCD calculations, Ref.[5]
g) LMTO-ASA calculations, Ref.[28]
h) Full-potential LAPW total energy calculations, Ref.[24]
i) Full-potential LAPW, Ref.[32]
j) Full-potential LMTO calculations, Ref.[34]
k) Full-potential LAPW calculations, Ref [36]
l) Experiment, Ref.[38]
m) Experiment, Rep.[40]

Table 5: Experiment and theoretical top layer relaxation for the low-index surface 3 Bcc metals.

Element	Crystal face(hkl)	Relaxation AECT	Semi empirical calculations	First principle calculations	Expt. Values
Mo	(100)	-4.44	-6.9[c], -3.3[b]	-4.36[e], -9.0[f], -31.05[y], -11.0[y]	-2.8[p], -9.0[r], 11.5[s] -6.0[s]
	(110)	-317	-3.3[c], -3.3[b]	-1.56[e], -3.9[f], -4.74[g]	-1.5[p], -1.6[q]
	(111)	-11.00	-19.7[c], -14.0[b]		
W	(100)	-3.80	-3.5[C], -3.2[b], -2.1[d]	-5.5[h], -5.9[i], -5.7[j]	-4.4 to -10.0[g]
	(110)	-2.53	-1.4[c], -3.0[b], -2.1[d]	-3.3[h], -3.6[l]	-3.1[l], -3.0[m] <I2I>[z], -0[aa]
	(111)	-9.87	-16.3[c], -13.2[b] -3.0[d]		
Fe	(100)	-5.59	-1.1[b] -5.07[d]	-6.0[h]	-1.5[e] -1.4[t] -0.2[b]
	(110)	-4.20	-1.5[b] -5.07[d]		+0.5[k], 0[d]
	(111)		-10.5[b] -5.36[d]		-15.4[k], -16.9[b]

CHAPTER FIVE

5.1. FINDINGS, CONCLUSION AND SUGGESTION FOR FURTHER STUDIES

5.1. FINDINGS

We have successfully extended the surface energy results of the AECT method first proposed by Zypman and Ferrante (15) for Fcc only to Bcc metals.

The calculated surface energies of Bcc metals are uniformly larger than the corresponding results from other semi-empirical work, it has been found that the surface energy results from this study consistently support the trend, $\sigma 110 < \sigma 111 < \sigma 100$ for Bcc metals which then shows that the densest packed Bcc (110) surface posses the lowest energy

5.2 CONCLUTION

We have in this study employed the new analytical equivalent theory method to provide a set of surface energy for bcc metals. In this work three surfaces were considered for 3 bcc metals. These are the (100), (110) and (111) surfaces. The surface energies of the 3 Bcc metals were found to be in good agreement with the available first-principle calculations and experimental data.

5.3 SUGGESTION FOR FURTHER STUDIES

This work should be extended to other available Bcc metals

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