

COMPARISON OF THE CALCULATED SURFACE ENERGY OF METAL USING PSEUDOPOTENTIAL MODEL WITH OTHER CALCULATED METHODS AND EXPERIMENTAL VALUES

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ABSTRACT

The Surface energy γ is the surface free energy per unit area of a particular crystal. The low index surface energies of metal surface was calculated for sixty (60) metals in the periodic table using the pseudopotential model proposed by Perdew(1995). The results obtained were compared with the Full Charged density (FCD), Full Potential calculation as well as the Experimental Values. Results obtained shows that the calculated results agreed well with the other works as well as experimental values.

KEYWORDS: *Metal Surface Energy, Fully Charged Density (FCD), Full Potential (FP), Psuedopotential Model (SJM)*

INTRODUCTION

The Surface energy γ is the surface free energy per unit area of a particular crystal. It is also the energy required to create a new unit area. Surface energy of solids is one of the important electronic properties of solid surfaces. It determines the equilibrium shape of mezosopic crystals. Surface energy plays an important role in faceting, roughening and crystal growth phenomena (Vitoset.al 1998). Surface energy controls a wide range of phenomenon such as stress for brittle fracture, the rate of sintering and the growth rate during particle coarsening. Consequently, a lot of efforts have been made to study surface energy theoretically and experimentally (Huntigton, 1951), (Lang and Kohn 1970).

Lang and Kohn, (1970) introduced the exchange and correlation contributions using local density approximation. The surface energy is the sum of four terms: kinetic, electrostatic, exchange and correlation terms. Lang and Kohn (1970) showed that the surface energy of the jellium was negative at high-electron density. The surface energy was negative because of the large contribution of the kinetic surface energy. Harris and Jones (1974) used the infinite barrier model to calculate the surface energy of metals. The infinite barrier model gave surface kinetic energy that is positive unlike the results of Kohn and Lang (1970). In the infinite barrier model, the sum of the kinetic, exchange and correlation energy is dominated by the large kinetic energy. Mahan, (1975) used variational calculation of the jellium model of a metal surface to obtain results that prove that the results of Lang and Kohn (1970) are better than those reported using the infinite barrier model. Monnier and Perdew (1978) improved the work of Lang and Kohn (1970) by treating the ground state of the metal surface varitionally and self-consistently. The results of Monnier and Perdew (1978) revealed that the surface energy of some metals is lower than the values predicted by Lang and Kohn (1970). Zang et al., (1990) used the self-consistent Langreth-Mehl calculations for metal surfaces to calculate the surface energy the surface energy of most densely closed

packed faces of face centred cubic metals. The result of the self-consistent Langreth –Mehl calculations was close to experimental values for some of the metals. Skriver and Rosengaard (1992) used the ab initio method to calculate the surface for face centred cubic (fcc), body centred cubic (bcc) and hexagonal closed packed (hcp) metals. There was discrepancy between the ab initio calculated surface energy and experimental values. Shore and Rose (1991) proposed the theory of idea metals and used the theory to predict the trends in surface energies among other properties. Methfesselet. *al* (1992) have used the full potential linear muffin-tin orbitals (LMTO) method to investigate the trend Kaijna (1993) calculated the surface energy of Li, Na, K, Rb,Cs, Al, Pb, Zn, and Mg using the structureless pseudopotential method. The results of this calculation were close to experimental values. Zanget *al.*, (2006) calculated the surface energy of bcc transition metals using the second nearest neighbour modified embedded atoms method for 24 different faces of bcc metals. Their results for the bcc metals were consistent with experimental values for the (110), (100) and (111) faces and they proposed that for the bcc metals, the (110) texture should be favourable for thin film formation.

In this work, the surface energy of faces (111), (100), (110), (211), (310), (0001), $(10\bar{1}0)_A$, and $(10\bar{1}0)_B$ were calculated using the pseudopotential model for metals with body centred cubic (bcc), face centred cubic (fcc) and hexagonal closed packed (hcp) as reference points. This was achieved with the use of MATLAB and equation editor for the smooth running of the equation. This model requires less computer resource, unlike the self-consistent method of Monnier and Perdew (1978) and the ab initio surface calculation of Skriver and Rosengaard (1992). The results obtained were compared with the Full Charged density (FCD) results (Vitoset.*al* 1998), Full Potential (FP) calculation results (Kokkoet.*al* 1996), other works as well as the available Experimental Values. The variation of the calculated surface energies of metals will be investigated.

METHODOLOGY

The surface energy of a metal is the energy required to create a new unit area (Lang & Kohn 1970). The energy functional of a stabilized jellium model is (Kiejna, 1993)

$$E[n, n_+] = E_J[n, n_+] + (E_m + W_R) \int d^3r m_+(r) + \langle \delta v \rangle_{sc} \int d^3r \theta(r) [n(r) - n_+(r)] \quad (1)$$

where E_J is the jellium total energy functional given as

$$E_J = T_s[n] + E_{xc}[n] + \frac{1}{2} \int d^3r \phi([n, n_+], r) [n(r) - n_+(r)] \quad (2)$$

$T_s[n]$ and $E_{xc}[n]$ are the respective kinetic and exchange-correlation energies. $\phi([n, n_+], r)$ is the electrostatic potential of the jellium. E_m is the Madelung energy, W_R is the short range repulsive potential of the ionic potential and $\theta(r)$ is the unit function. For a metal surface, the second term in equation (1) does not contribute to the energy since it is purely bulk.

The surface energy is conventionally decomposed into the kinetic, electrostatic, exchange-correlation and the pseudopotential terms.

$$\sigma = \sigma_s + \sigma_{es} + \sigma_{xc} + \sigma_{ps} \quad (3)$$

Where σ_s is the kinetic surface energy, σ_{es} is the surface electrostatic energy, σ_{xc} is the exchange-correlation surface energy and σ_{ps} is the pseudopotential surface energy terms.

$$\sigma_s = \frac{1}{2\pi^2} \int_0^{k_f} dk k^3 \left(n_k - \frac{\pi}{4} \right) - \int_{-\infty}^{\infty} dx n(x) [V_{eff}(x) - V_{eff}(-\infty)] \quad (4)$$

Where n_k is the phase-shift and V_{eff} is the effective potential in the stabilized jellium model. For the electrostatic surface energy

$$\sigma_{es} = \frac{1}{2} \int_{-\infty}^{\infty} dx \phi(x) [n(x) - n_+(x)] \quad (5)$$

and the exchange-correlation components is

$$\sigma_{xc} = \int_{-\infty}^{\infty} dx n(x) \left\{ \varepsilon_{xc}[n(x)] - \varepsilon_{xc}[\bar{n}] \right\} \quad (6)$$

Where ε_{xc} is the exchange -correlation energy in the local density approximation of the density functional theory, $n(x)$ is the electron density and n_+ is the density of the positively charged background.

The pseudopotential surface energy is the surface energy arising from the stabilization of the jellium and it is

$$\sigma_{ps} = \langle \delta v \rangle_{ws} \int_{-\infty}^0 dx [n(x) - n_+(x)] \quad (7)$$

Where $\langle \delta v \rangle_{ws}$ is the stabilization potential given as (Perdew *et al.*, 1990)

$$\langle \delta v \rangle_{ws} = -\frac{d}{dn} \left[t_s(\bar{n}) + \varepsilon_{xc}(\bar{n}) \right] \quad (8)$$

Hence

$$\sigma = \sigma_{jellium} + \sigma_{ps} \quad (9)$$

For any exposed crystal face, the surface energy is

$$\sigma = \sigma_{jellium} + \sigma_{ps} + \frac{3z}{10r_0} \left[1 - \frac{5}{12} \left(\frac{d}{r_0} \right)^2 \right] \quad (10)$$

Where $r_0 = z^{1/3} r_s$, r_s is electron gas parameter defined through the relation, $n_{ave} = 3/4\pi r_s^3$ and d is inter-planar spacing.

Brajczewska et al., (2001) based on the stabilized jellium model proposed the expression for the different contributions to the surface energy as

$$\sigma_s = \frac{-1.554 \times 10^5}{r_s^5} \quad (11)$$

$$\sigma_{xc} = \frac{3.001 \times 10^4}{r_s^3} \quad (12)$$

$$\sigma_{es} = \frac{1.160 \times 10^4}{r_s^4} \quad (13)$$

$$\sigma_{ps} = \frac{2.584 \times 10^5}{r_s^7} \quad (14)$$

While that of the surface energy is

$$\sigma = \frac{8134}{r_s^{2.6}} \quad (15)$$

Equations (11), (12), (13) and (14) were used to calculate the different components of the surface energy and the surface energy based on equation (9). Equation (15) was also used to calculate the surface energy. The face dependence of surface energy for body centred cubic (bcc) and face centred cubic (fcc), Hexagonal closed packed (hcp), sc^* and bct^* metals was calculated using equation (10). The calculated surface energy using all the equations was compared with experimental values.

RESULTS AND DISCUSSIONS

The surface energies of metals were calculated and compared with the results obtained by Vitos et.al (1998) that used the Full Charged density (FCD), which was derived from density functional theory (DFT) in the local density approximation (LDA) as well as generalized gradient approximation (GGA). The present surface energy results are shown in table 1 to table 7 in $eV \text{ atom}^{-1}$ as well as Jm^{-2} . For monovalent metals, the SJM closely agrees perfectly with the Experimental, FCD and FP results. The surface energy anisotropy of the monovalent metals are in good agreement. For the divalent metals, it was discovered that the surface energy of the second most closed packed surface is consistently lower than that of the most closed packed surface. SJM is more accurate when it comes to simple metals. In the early hcp transition metals, the surface energy exhibit a weak orientation dependence and for those elements we find the facets $(10\bar{1}0)$ are more stable than the most close packed (0001) facets. For the 5f metals, the agreement between the experimentally derived and the theoretical values is very good.

This work calculated a database of low index surface energies for 60 metals which may be used as a starting point for the understanding of a wide range of surface phenomenon including faceting, roughening, crystal growth, surface segregation and equilibrium shape of mesoscopic crystals. The comparison with Experimental values, FCP and the FP shows that the SJM is in better agreement with the experimental for so many metals than results of some other works.

Table 1: Compared Calculated SJM (Pseudopotential) Surface Energies Values for Monovalent Sp Metals with FCD Method in the CGA, FP Calculation and Experimental Data

Metal r_s (a.u)	Structure (a (Å))	Surface	FCD (eV atom ⁻¹)	FCD (J m ⁻²)	FP (J m ⁻²)	This Work SJM (J m ⁻²)	Experiment (J m ⁻²)
Li 3.25	bcc (3.431)	(110)	0.289	0.556	0.545 ^a	0.536	0.522 ^b , 0.525 ^c
		(100)	0.383	0.522	0.506 ^a	0.514	
		(111)	0.750	0.590	0.623 ^a	0.598	
Na 3.93	bcc (4.197)	(110)	0.197	0.253		0.249	0.261 ^b , 0.260 ^c
		(100)	0.290	0.264		0.257	
		(111)	0.546	0.287		0.289	
K 4.86	Bcc (5.300)	(110)	0.167	0.135		0.140	0.145 ^b , 0.130 ^c
		(100)	0.249	0.142		0.141	
		(111)	0.462	0.152		0.145	
Rb 5.20	Bcc (5.714)	(110)	0.150	0.104		0.110	0.117 ^b , 0.110 ^c
		(100)	0.229	0.112		0.112	
		(111)	0.417	0.118		0.116	
Cs 5.63	Bcc (6.264)	(110)	0.142	0.082		0.080	0.095 ^b , 0.095 ^c
		(100)	0.228	0.093		0.090	
		(111)	0.390	0.092		0.092	
Fr 6.12	Bcc (6.320)	(110)	0.122	0.069		0.700	
		(100)	0.202	0.081		0.702	
		(111)	0.346	0.080		0.705	

Table 2: Compared Calculated SJM (Pseudopotential) Surface Energies Values for Divalent Sp Metals with FCD Method in the CGA, FP Calculation and Experimental Data

Metal r_s (a.u)	Structure (a (Å))	Surface	FCD (eV atom ⁻¹)	FCD (J m ⁻²)	FP (J m ⁻²)	This Work SJM (J m ⁻²)	Experiment (J m ⁻²)
Ca 3.27	fcc (5.624)	(111)	0.484	0.567	0.545 ^a	0.550	0.502 ^a , 0.490 ^b
		(100)	0.535	0.542	0.506 ^a	0.560	
		(110)	0.811	0.582	0.623 ^a	0.580	
Sr 3.57	fcc (6.169)	(111)	0.440	0.428		0.422	0.419 ^a , 0.410 ^b
		(100)	0.484	0.408		0.410	
		(110)	0.725	0.432		0.430	
Ba 3.71	bcc (5.289)	(110)	0.464	0.376		0.370	0.380 ^a , 0.370 ^b
		(100)	0.616	0.353		0.350	
		(111)	1.199	0.397		0.390	
Ra 3.92	bcc (5.372)	(110)	0.377	0.296		0.289	
		(100)	0.515	0.286		0.285	
		(111)	1.010	0.324		0.300	
Eu 2.98	bcc (4.757)	(110)	0.484	0.485		0.430	0.450 ^b ,
		(100)	0.653	0.463		0.460	
		(111)	1.282	0.524		0.525	
Yb 2.99	fcc (5.697)	(111)	0.423	0.482		0.488	0.500 ^b
		(100)	0.484	0.478		0.477	
		(110)	0.721	0.503		0.499	
Be 1.88	hcp (2.236)	(0001)	0.495	1.834	1.924 ^c	1.822	1.628 ^a , 2.700 ^b
		(10 $\bar{1}$ 0) _A	1.083	2.126	2.1 ^d	1.999	
		(10 $\bar{1}$ 0) _B	1.626	3.192		2.500	

Table 2: Contd.,

Mg 2.66	hcp (3.196)	(0001) (10 $\bar{1}$ 0) _A (10 $\bar{1}$ 0) _B	0.437 0.814 1.072	0.792 0.782 1.030	0.641 ^c	0.800 0.798 1.001	
Zn 2.31	hcp (2.684, <i>c/a</i> = 1.86)	(0001)	0.385	0.989		0.978	0.993 ^a , 0.990 ^b
Cd 2.59	hcp (3.061, <i>c/a</i> = 1.89)	(0001)	0.300	0.593		0.600	0.762 ^a , 0.740 ^b
Hg 2.65	Hcp* (3.528)	(0001)	0.111	0.165		0.215	0.605 ^a , 0.575 ^b

Table 3: Compared Calculated SJM (Pseudopotential) Surface Energies Values for Group III-IVA Metals with FCD Method in the CGA, FP Calculation and Experimental Data

Metal <i>r_s</i> (a.u)	Structure (a (Å))	Surface	FCD (eV atom ⁻¹)	FCD (J m ⁻²)	FP (J m ⁻²)	This Work SJM (J m ⁻²)	Experiment (J m ⁻²)
Al 2.07	fcc (4.049)	(111) (100) (110)	0.531 0.689 0.919	1.199 1.347 1.271	0.939 ^a 1.081 ^a 1.090 ^a	1.112 1.201 1.230	1.143 ^b , 1.160 ^c
Ga 2.19	Bct* (3.018, <i>c/a</i> = 1.58)	(001) (110) (100)	0.376 0.507 0.695	0.661 0.797 0.773		0.665 0.790 0.770	0.881 ^b , 1.100 ^c
In 2.41	bct (3.352, <i>c/a</i> = 1.52)	(001) (110) (100)	0.342 0.422 0.632	0.488 0.560 0.592		0.501 0.550 0.596	0.700 ^b , 0.675 ^c
Tl 2.48	hcp (3.714)	(0001) (10 $\bar{1}$ 0) _A (10 $\bar{1}$ 0) _B	0.221 0.494 0.529	0.297 0.352 0.377		0.300 0.355 0.377	0.602 ^b , 0.575 ^c
Sn 2.22	bct (3.187, <i>c/a</i> = 1.83)	(001) (110) (100)	0.387 0.509 0.716	0.611 0.620 0.616		0.620 0.63 0.619	0.709 ^b , 0.675 ^c
Pb 2.28	fcc (5.113)	(111) (100) (110)	0.226 0.307 0.513	0.321 0.377 0.445	0.496 ^d 0.592 ^d	0.478	0.593 ^b , 0.600 ^c
Sb 2.14	Sc* (3.102)	(100) (110)	0.365 0.560	0.608 0.659		0.607 0.688	0.597 ^b , 0.535 ^c
Bi 2.25	Sc* (3.257)	(100) (110)	0.356 0.507	0.537 0.541		0.542 0.545	0.489 ^b , 0.490 ^c
Po 2.20	sc (3.349)	(100) (110)	0.306 0.370	0.437 0.373		0.438 0.398	

Table 4: Compared Calculated SJM (Pseudopotential) Surface Energies Values for 3d Metals with FCD Method in the CGA, FP Calculation and Experimental Data

Metal r_s (a.u)	Structure (a (Å))	Surface	FCD (eV atom ⁻¹)	FCD (J m ⁻²)	FP (J m ⁻²)	This Work SJM (J m ⁻²)	Experiment (J m ⁻²)
Sc 3.32	hcp (3.300)	(0001)	1.080	1.834		1.528	1.275 ^a
		(10 $\bar{1}0$) _A	1.694	1.526		1.560	
		(10 $\bar{1}0$) _B	2.011	1.812		1.712	
Ti 1.92	hcp (2.945)	(0001)	1.234	2.632	2.194 ^b	2.574	1.989 ^c , 2.100 ^a
		(10 $\bar{1}0$) _A	2.224	2.516		2.434	
		(10 $\bar{1}0$) _B	2.435	2.754		2.645	
V 1.64	bcc (3.021)	(110)	1.312	3.258	3.18 ^d	3.001	2.622 ^c , 2.550 ^a
		(100)	1.725	3.028		2.989	
		(211)	2.402	3.443		3.220	
		(310)	2.921	3.244		3.435	
		(111)	3.494	3.541		3.540	
Cr 1.86	bcc* (2.852)	(110)	1.258	3.505		3.450	2.354 ^c , 2.300 ^a
		(100)	2.020	3.979		3.978	
		(211)	2.420	3.892		3.873	
		(310)	3.030	3.775		3.774	
		(111)	3.626	4.123		3.989	
Mn 2.14	fcc* (3.529)	(111)	1.043	3.100		2.999	1.543 ^c , 1.600 ^a
Fe 1.86	bcc (3.001)	(110)	0.978	2.430		2.418	2.417 ^c , 2.475 ^a
		(100)	1.265	2.222		2.300	
		(211)	1.804	2.589		2.519	
		(310)	2.153	2.393		2.399	
		(111)	2.694	2.733		2.745	
Co 2.07	hcp (2.532)	(0001)	0.961	2.775		2.600	2.522 ^c , 2.550 ^a
		(10 $\bar{1}0$) _A	1.982	3.035		2.989	
		(10 $\bar{1}0$) _B	2.476	3.791		3.219	
Ni 2.07	fcc (3.578)	(111)	0.695	2.011		2.101	2.380 ^c , 2.450 ^a
		(100)	0.969	2.426		2.231	
		(110)	1.337	2.368		2.343	
Cu 2.12	fcc (3.661)	(111)	0.707	1.952	1.94 ^e 1.802 ^f	1.850	1.790 ^c , 1.825 ^a
		(100)	0.906	2.166			
		(110)	1.323	2.237			

Table 5: Compared Calculated SJM (Pseudopotential) Surface Energies Values for 4d Metals with FCD Method in the CGA, FP Calculation and Experimental Data

Metal r_s (a.u)	Structure (a (Å))	Surface	FCD (eV atom ⁻¹)	FCD (J m ⁻²)	FP (J m ⁻²)	This Work SJM (J m ⁻²)	Experiment (J m ⁻²)
Y 2.61	hcp (3.638)	(0001)	1.077	1.506		1.234	1.125 ^a
		(10 $\bar{1}0$) _A	1.676	1.243		1.245	
		(10 $\bar{1}0$) _B	2.059	1.527		1.501	
Zr 2.11	hcp (3.248)	(0001)	1.288	2.260	2.044 ^b , 1.729 ^c	2.003	1.989 ^c , 2.100 ^a
		(10 $\bar{1}0$) _A	2.269	2.111		2.121	
		(10 $\bar{1}0$) _B	2.592	2.411		2.198	
Nb 2.13	bcc (3.338)	(110)	1.320	2.685	2.36 ^e , 2.9 ^f 2.86 ^e , 3.1 ^f	2.675	2.655 ^d , 2.700 ^a
		(100)	1.987	2.858		2.785	
		(211)	2.410	2.829		2.800	
		(310)	3.145	2.861		2.812	
		(111)	3.668	3.045		2.898	

Table 5: Contd.,

Mo 1.84	bcc (3.173)	(110)	1.534	3.454	3.14 ^e , 3.52 ^e	3.124	2.907 ^d , 3.000 ^a
		(100)	2.410	3.837		3.342	
		(211)	2.738	3.600		3.455	
		(310)	3.601	3.625		3.501	
		(111)	4.068	3.740		3.567	
Tc 1.97	hcp (2.767)	(0001)	1.527	3.691		3.400	3.150 ^a ,
		(10 $\bar{1}$ 0) _A	3.040	3.897		3.513	
		(10 $\bar{1}$ 0) _B	3.893	4.989		3.975	
Ru 1.93	hcp (2.723)	(0001)	1.574	3.928	3.0 ^g , 4.3 ^g	3.261	3.043 ^d , 3.050 ^d
		(10 $\bar{1}$ 0) _A	3.201	4.236		3.585	
		(10 $\bar{1}$ 0) _B	3.669	4.856		3.989	
Rh 1.95	fcc (3.873)	(111)	1.002	2.472	2.53 ^e 2.81 ^e , 2.65 ^h 2.592 ⁱ 2.88 ^e	2.500	2.659 ^d , 2.700 ^a
		(100)	1.310	2.799		2.576	
		(110)	1.919	2.899		2.670	
Pd 2.38	Fcc (3.985)	(111)	0.824	1.920	1.64 ^e 1.86 ^e , 2.3 ^f , 2.130 ^j 1.97 ^e , 2.5 ^f	1.980	2.003 ^d , 2.050 ^d
		(100)	1.152	2.326		2.001	
		(110)	1.559	2.225		2.198	
Ag 2.89	fcc (4.179)	(111)	0.553	1.172	1.21 ^e 1.21 ^e , 1.3 ^f , 1.27 ^k 1.26 ^e , 1.4 ^f	1.200	1.246 ^d , 1.250 ^a
		(100)	0.653	1.200		1.201	
		(110)	0.953	1.238		1.240	

Table 6: Compared Calculated SJM (Pseudopotential) Surface Energies Values for 5d Metals with FCD Method in the CGA, FP Calculation and Experimental Data

Metal r _s (a.u)	Structure (a (Å))	Surface	FCD (eV atom ⁻¹)	FCD (J m ⁻²)	FP (J m ⁻²)	This Work SJM (J m ⁻²)	Experiment (J m ⁻²)
La 2.89	Hcp* (3.873)	(0001)	0.909	1.121		1.130	1.020 ^a
		(10 $\bar{1}$ 0) _A	1.389	0.915		0.998	
		(10 $\bar{1}$ 0) _B	1.690	1.106		1.001	
Lu 2.87	hcp (3.566)	(0001)	1.102	1.604		1.300	1.225 ^a
		(10 $\bar{1}$ 0) _A	1.845	1.424		1.345	
		(10 $\bar{1}$ 0) _B	2.093	1.616		1.462	
Hf 2.43	hcp (3.237)	(0001)	1.400	2.472		2.203	2.193 ^b , 2.150 ^a
		(10 $\bar{1}$ 0) _A	2.471	2.314		2.321	
		(10 $\bar{1}$ 0) _B	2.892	2.709		2.435	
Ta 2.48	bcc (3.354)	(110)	1.531	3.084		2.987	2.902 ^b , 3.150 ^a
		(100)	2.174	3.097		2.998	
		(211)	2.799	3.256		3.001	
		(310)	2.485	3.139		3.124	
		(111)	4.201	3.455		3.319	
W 1.62	bcc (3.196)	(110)	1.806	4.005	4.78 ^c	3.532	3.265 ^b , 3.675 ^a
		(100)	2.955	4.635		3.598	
		(211)	3.261	4.177		3.670	
		(310)	4.338	4.303		3.745	
		(111)	4.916	4.452		3.779	
Re 2.01	hcp (2.797)	(0001)	1.781	4.214		3.596	3.626 ^a , 3.600 ^b
		(10 $\bar{1}$ 0) _A	3.689	4.628		3.896	
		(10 $\bar{1}$ 0) _B	4.770	5.985		4.029	
Os 1.97	hcp (2.752)	(0001)	1.869	4.566		3.670	3.439 ^b , 3.450 ^a
		(10 $\bar{1}$ 0) _A	3.874	5.021		3.699	
		(10 $\bar{1}$ 0) _B	4.595	5.955		4.192	

Table 6: Contd.,

Ir 1.87	hcp (3.907)	(111)	1.225	2.971		2.979	3.048 ^b , 3.000 ^a
		(100)	1.772	3.722		3.194	
		(110)	2.428	3.606		3.123	
Pt 2.0	fcc (4.019)	(111)	1.004	2.299	2.067 ^d	2.300	2.489 ^b , 2.475 ^a
		(100)	1.378	2.734		2.359	
		(110)	2.009	2.819		2.415	
Au 2.39	fcc (4.198)	(111)	0.611	1.283	1.04 ^e	1.478	1.506 ^b , 1.500 ^a
		(100)	0.895	1.627		1.498	
		(110)	1.321	1.700		1.597	

Table 7: Compared Calculated SJM (Pseudopotential) Surface Energies Values for 5f Metals with FCD Method in the CGA, FP Calculation and Experimental Data

Metal r_s (a.u)	Structure (a (Å))	Surface	FCD (eV atom ⁻¹)	FCD (J m ⁻²)	FP (J m ⁻²)	This work SJM (J m ⁻²)	Experiment (J m ⁻²)
Ac 2.89	fcc (5.786)	(111)	0.786	0.868		0.879	
		(100)	0.764	0.732		0.798	
		(110)	1.006	0.681		.0691	
Th 2.98	fcc (5.188)	(111)	1.073	1.476		1.489	1.500 ^a
		(100)	1.233	1.468		1.469	
		(110)	1.722	1.450		1.487	
Pa 2.72	bct (3.986, c/a = 0.82) Fcc* (4.784)	(110)	1.648	2.902		2.900	
		(100)	2.075	2.584		2.694	
		(001)	2.638	2.661		2.653	
		(111)	1.424	2.302		2.321	
U 2.55	Fcc* (4.634)	(111)	1.367	2.36		2.032	1.939 ^b , 1.900 ^a
Np 2.50	Fcc* (4.580)	(111)	1.252	2.208		2.213	
Pu 2.54	Fcc* (4.513)	(111)	1.104	2.007		2.000	2.000 ^a

^aPseudopotential Ref [Kokkoet.al 1996]

^bExperimental Ref [Tyson and Miller 1977]

^cExperimental Ref [de Boar et.al 1988]

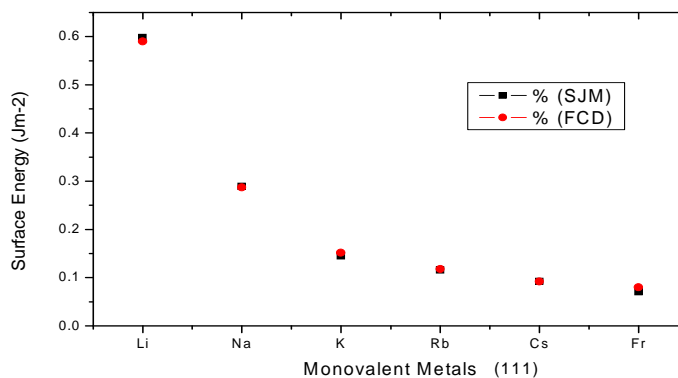


Figure 1: Comparison of the FCD and SJM Surface Energy Values for (111) Monovalent Sp Metals.

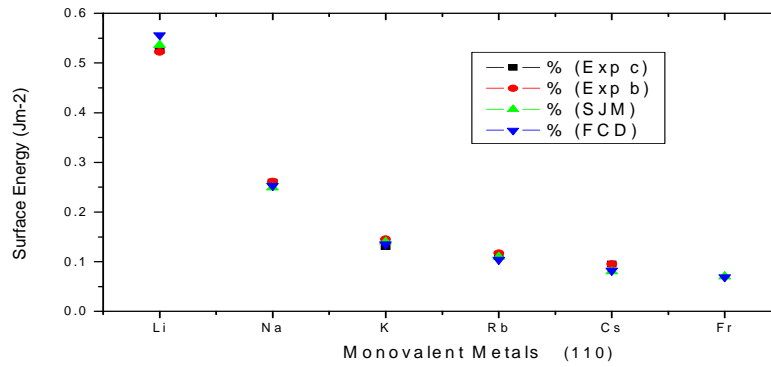


Figure 2: Comparison of the FCD and SJM Surface Energy Values for (110) Monovalent Sp Metals.

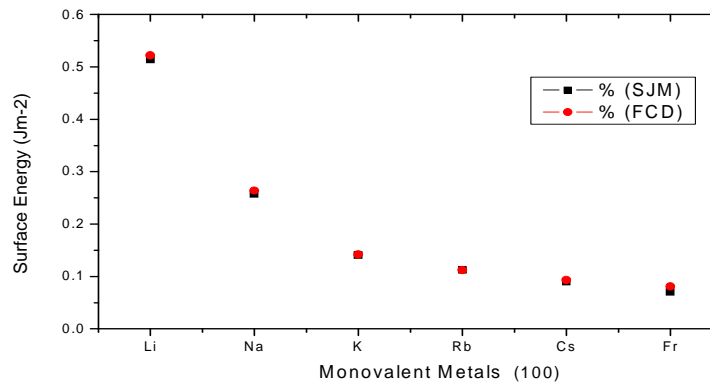


Figure 3: Comparison of the FCD and SJM Surface Energy Values for (100) Monovalent Sp Metals.

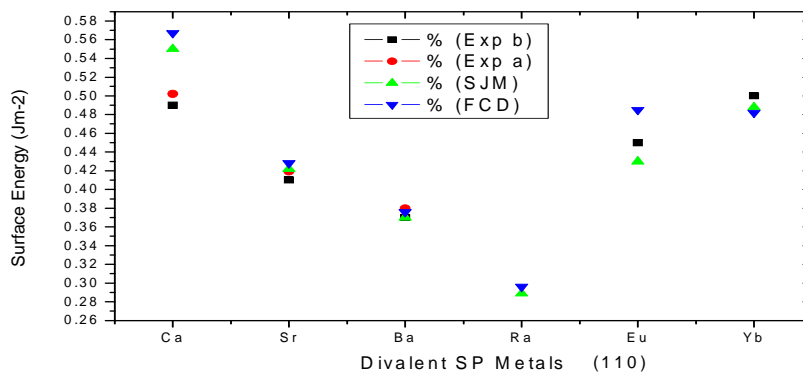


Figure 4: Comparison of the FCD and SJM Surface Energy Values for (110) Divalent Sp Metals.

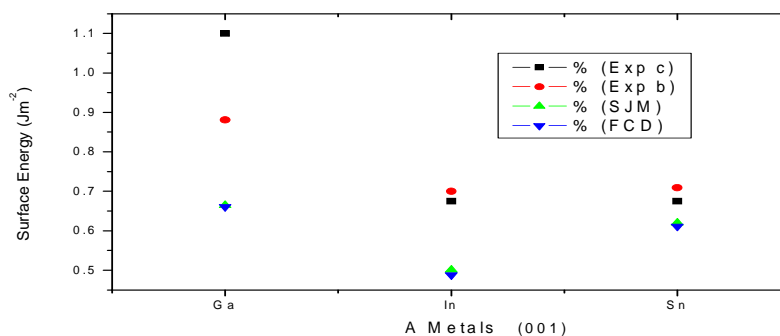


Figure 5: Comparison of the FCD and SJM Surface Energy Values for (001) Group III-VIA Sp Metals.

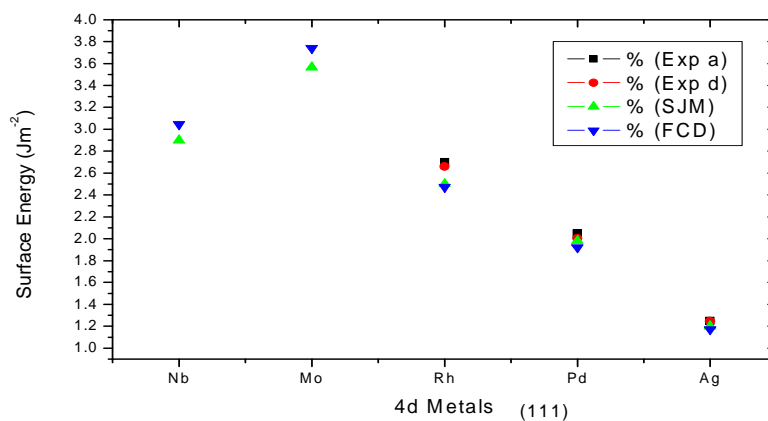


Figure 6: Comparison of the FCD and SJM Surface Energy Values for 4d Metals for (111).

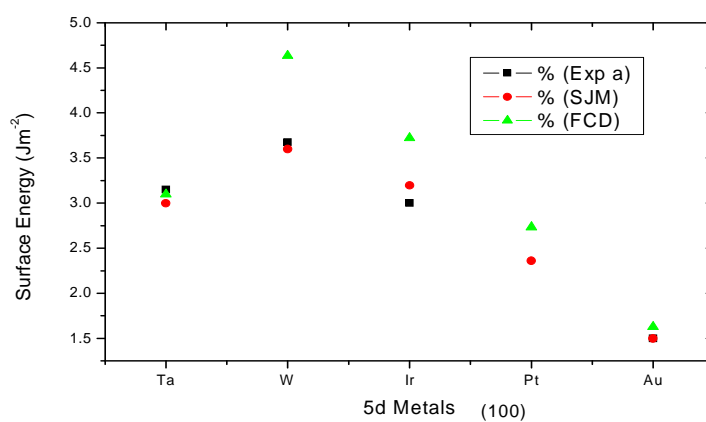


Figure 7: Comparison of the FCD and SJM Surface Energy Values for 4.5d Metals for (100).

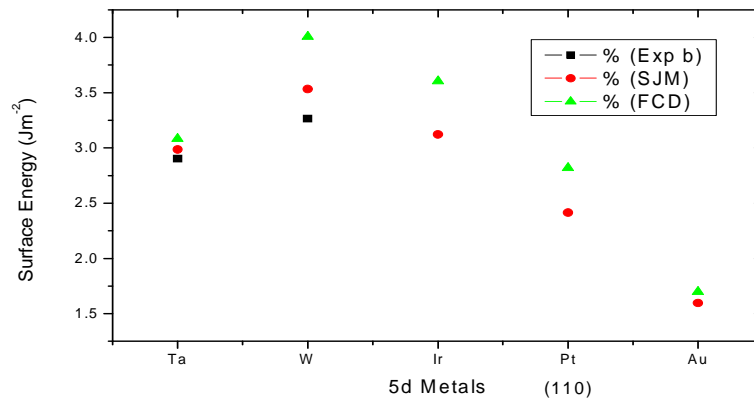


Figure 8: Comparison of the FCD and SJM Surface Energy Values for 4.5d Metals for (110).

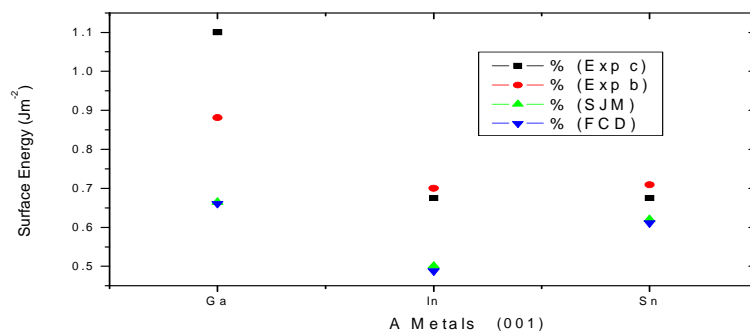


Figure 9: Comparison of the FCD and SJM Surface Energy Values for 5f Metals for (001).

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