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Abstract
A simple formula without any free parameter is established to estimate surface
energies of elemental metals of low-index surfaces, which is developed by
modifying the classic broken-bond rule. The predicted results of the formula
for 52 A1–A4 and sc elemental crystals are in agreement with experimental
results and the first-principles calculations although deviations are present for
several divalent sp metals.

1. Introduction

The surface energy γ is usually defined as the difference between the free energy of the surface
and that of the bulk or simply as the energy needed to split a solid in two along a plane, which is
one of the basic quantities to understand the surface structure, reconstruction, roughening and
relaxation [1–3]. Despite its importance, the γ value is difficult to determine experimentally.
Most of these experiments are performed at high temperatures where the surface tension of the
liquid is measured, which is extrapolated to 0 K. This kind of experiment contains uncertainties
of unknown magnitude [4, 5] and only corresponds to the γ value of an isotropic crystal [6].
Note that many published data determined by the contact angle of metal droplets or from peel
tests disagree each other, which can be induced by the presence of impurities or by mechanical
contributions, such as dislocation slip or the transfer of material across the boundary [7]. In
addition, there are hardly any experimental data on the more open surfaces except for the classic
measurements on Au, Pb and In [8] to our knowledge. Therefore, a theoretical determination
of γ values especially for open surfaces is of vital importance.

In recent years there have been several attempts to calculate γ values of metals using either
ab initio techniques [9–11] with tight-binding (TB) parametrizations [12] or semi-empirical
methods [13]. γ values, work functions and relaxation for the whole series of body centred

cubic (A2) and face centred cubic (A1) 4d transition metals were first studied [9] using the full-potential (FP) linear muffin-tin orbital (LMTO) method in conjunction with the local-spin density approximation to the exchange–correlation potential [14–16]. In the same spirit, γ values and the work functions of the most elemental metals including the light actinides have been found by the Green function with LMTO method [10, 11, 17, 18]. Recently, the full-charge density (FCD) Green function LMTO technique in the atomic-sphere approximation (ASA) with the generalized gradient approximation (GGA) has been utilized to construct a large database that contains γ values of low-index surfaces of 60 elements in the periodic table [6, 19–22]. The results denote a mean deviation of 10% for the 4d transition metals from FP methods [23]. This database in conjunction with the pair-potential model [24] has been further extended to estimate the formation energy of monatomic steps on low-index surfaces for an ensemble of the A1 and A2 metals [25].

On the other side, the traditional broken-bond model is again suggested to estimate γ values of the transition metals and the noble metals with different facets [8, 26, 27]. The simplest approach to get a rough estimation of γ values at $T = 0$ K is to determine the broken-bond number $Z_{(hkl)}$ for creating a surface area by cutting a crystal along certain crystallographic plane with a Miller index (hkl). $Z_{(hkl)} = Z_B - Z_S$ where Z_S is the coordination number (CN) of surface atoms and Z_B the corresponding bulk one. Multiplying this number with the cohesion energy per bond E/Z_B for the non-spin-polarized atom at 0 K, γ is determined by [28]

$$\gamma = (1 - Z_S/Z_B)E. \tag{1}$$

In equation (1), E is independent of crystalline structure as a first-order approximation since energy differences between solid structures are several orders of magnitude smaller than E for any structure when the bond type remains unaltered. The broken-bond rule seems to contradict basic knowledge about the electronic structure since E in general does not scale linearly with Z_S. Nevertheless, the above estimation provides the order of magnitude of γ and shows a close relationship between γ and bond strength. The recent works support the above consideration in which the relaxation or the rearrangement of the electronic charge for noble metals does not practically lead to a change of the remaining bonds when one bond is broken; namely, the energy needed to break a bond is independent of the surface orientation [8, 27]. Although no verification from experiments or from *ab initio* methods exists, such a rule has been assumed to describe γ values of A1 elements [8].

Since the bond strength becomes stronger for an atom with a smaller CN, this CN–bond-strength relation can be quantified using the TB approximation. In the second-moment approximation, the width of the local density of states on an atom scales with Z_S, leading to an energy gain proportional to $\sqrt{Z_S}$ due to the lowing of the occupied states [26]. Neglecting repulsive terms, the energy per nearest neighbour is then proportional to $\sqrt{Z_S}$. By assuming that the total crystalline energy is a sum of contributions of all bonds of an atom, it follows that [26]

$$\gamma = [1 - (Z_S/Z_B)^{1/2}]E. \tag{2}$$

While equation (1) does not consider the variation of bond strength with CN, or relaxation, equation (2) is not complete because only attractive forces are taken into account [9]. Namely, equation (1) neglects while equation (2) overestimates the effect of relaxation on γ when γ is directly related to $Z_{(hkl)}$, which results in equation (1) being an acceptable concept for strongly covalent crystals while equation (2) is especially suitable for noble metals.

In this contribution, the above two models are improved to predict γ values of elements with different facets by suggesting an improved formula that is the arithmetic mean of the two formulae. Although this is a pragmatic interpolation approach rather than a new insight into fundamentals of surface energy, this single empirical formula can account for γ values

of 52 elements of different facets, which include the normal metals, group IV elements and transition metals. The formula predictions correspond to the experimental and the theoretical results.

2. Model

Although a direct utilization of equation (1) or (2) is reasonable, one of them cannot alone give satisfied predictions for γ values in comparison with the experimental and theoretical results [9]. To obtain a more general formula, as a first approximation, we arbitrarily assume that both equations (1) and (2) could make up the deficiency each other with the same weight to both formulae. Thus, γ values may be determined by an averaged effect of them without elaborate estimation on the relaxation energy,

$$\gamma = [2 - Z_S/Z_B - (Z_S/Z_B)^{1/2}]E/2. \tag{3}$$

Equation (3) implies that γ values still depend on the bond-broken rule although they are scaled by both Z_S and $\sqrt{Z_S}$.

In equation (3), Z_S can be determined according to the crystalline structure through determining $Z_{(hkl)}$ by a geometric consideration [29, 30]. For an A1 or A3 (hexagonal close-packing) structure, $Z_B = 12$; for an A2 lattice, although $Z_B = 8$ is taken according to the nearest-neighbour definition by some authors (probably the majority), others prefer to regard $Z_B = 14$ since the difference between the nearest-neighbour bond length and the next-nearest-neighbour bond length is small [31]. In our consideration, the latter is accepted. By assuming that the total energy of a surface atom is the sum of contributions from both the nearest-neighbour and the next-nearest-neighbour atoms, equation (3) should be rewritten for A2 metals after normalization.

$$\gamma = \{[2 - Z_S/Z_B - (Z_S/Z_B)^{1/2}] + \beta[2 - Z_S'/Z_B' - (Z_S'/Z_B')^{1/2}]\}E/(2+2\beta), \tag{4}$$

where the prime denotes the next-nearest CN on a surface and β shows the total bond strength ratio between the next-nearest neighbour and the nearest neighbour [32]. To roughly estimate the size of β, the Lennard-Jones (LJ) potential is utilized [32]. The potential is expressed as $u(r) = -4\varepsilon[(\lambda/r)^6 - (\lambda/r)^{12}]$ with ε being the bond energy and λ insuring $du(r)/dr_{(r=h)} = 0$, i.e. $\lambda = 2^{-1/6}h$ where h is the atomic distance in equilibrium and r is the atomic distance. For an A2 crystal, $h = \sqrt{3}a/2$ and $h' = a$, respectively. Let $r = a$, $\varepsilon' = 2/3\varepsilon$. Thus, $\beta = [(2/3) \times 6]/8 = 1/2$. Adding this value to equation (4),

$$\gamma = [3 - Z_S/Z_B - (Z_S/Z_B)^{1/2} - Z_S'/(2Z_B') - (Z_S'/(4Z_B'))^{1/2}]E/3. \tag{5a}$$

Note that the bonding of the LJ potential, which is utilized to justify the β value in equation (4), is different from the metallic bond in its nature. For instance, in an LJ bonded system, the surface relaxation is outwards whilst in the transition metals it is inwards. However, this difference leads to only a second-order error in our case and has been neglected.

The effect of next-nearest CN also occurs for simple cubic (sc) and diamond structure (A4) crystals because there are two and three times as the second neighbours as first neighbours, respectively. Similar to the above analysis, for sc crystals $\varepsilon' \approx \varepsilon/4$ with $h = a$ and $h' = \sqrt{2}a$. Thus, $\beta = [(1/4) \times 12]/6 = 1/2$, which is the same for A2 and thus equation (5a) can also hold for sc crystals. For A4, $\varepsilon' \approx \varepsilon/10$ with $h = a$ and $h' = \sqrt{8/3}a$. $\beta = [(1/10) \times 12]/4 = 3/10$. With this β value, equation (4) is rewritten as

$$\gamma = \{[26 - 10Z_S/Z_B - 10(Z_S/Z_B)^{1/2} - 3Z_S'/Z_B' - (9Z_S'/Z_B')^{1/2}]\}E/26. \tag{5b}$$

$Z_{(hkl)}$ can be determined by some known geometrical rules. For any surface of an A1 structure with $h \geqslant k \geqslant l$ [29, 30],

$$Z_{(hkl)} = 2h + k \qquad \text{for } h, k, l \text{ being odd,} \qquad (6a)$$

$$Z_{(hkl)} = 4h + 2k \qquad \text{for the rest.} \qquad (6b)$$

In a similar way, $Z_{(hkl)}$ for any surface of an A2 structure is determined with the consideration of the next-nearest CN [29],

$$Z_{(hkl)} = 2h + (h + k + l) \qquad \text{for } h + k + l \text{ being even,} \qquad (7a)$$

$$Z_{(hkl)} = 4h + 2(h + k + l) \qquad \text{for } h + k + l \text{ being odd} \quad \text{and} \quad h - k - l \geqslant 0, \quad (7b)$$

$$Z_{(hkl)} = 2(h + k + l) + 2(h + k + l) \qquad \text{for } h + k + l \text{ being odd} \quad \text{and} \quad -h + k + l > 0, \quad (7c)$$

where the second item of the right-hand side of equation (7) denotes the broken-bond number of the next-nearest neighbours. For sc crystals, $Z_{(hkl)}$ values of the nearest and the next-nearest atoms are 1 and 4 for the (100) surface as well as 2 and 5 for the (110) surface, respectively. For A4 crystals, $Z_{(hkl)}$ values of the nearest and the next-nearest atoms are 1 and 6 for the (110) surface.

For several surfaces of an A3 structure, $Z_{(hkil)}$ is obtained by [30]

$$Z_{(hkil)} = 4(h + k) + 3l \qquad \text{for (0001),} \qquad (8a)$$

$$Z_{(hkil)} = 4(h + k) + (8h + 4k)/3 \qquad \text{for } (10\bar{1}0), \qquad (8b)$$

where the first item of the right-hand side of equation (8) denotes the average number of basal broken bonds while the second item is that of non-basal broken bonds.

3. Results and discussion

Table 1 shows some used parameters in equations (3) and (5). Tables 2–4 give the predicted γ values for A1–A4 and sc crystals in terms of equations (3) and (5) where two sets of experimental results γ'' [4, 5] and the first principle calculations γ' [6] are also shown. Note that the experimental results are not orientation-specific but are averaged values of isotropic crystals. Thus, they should be close to those of the most close-packed surface.

For both noble and transition metals, our predictions agree nicely with the experimental results and FCD calculations as shown in tables 2–4 although our predictions for transition metals have slightly larger deviations than those for the noble metals due to the fact that their d bands are not fully filled and they present peaks at the Fermi level, which can slightly change from one surface orientation to the other and consequently the energy needed to break a bond also changes a little.

As shown in the tables, γ values of transition metals increase along an isoelectronic row where a heavier element has a larger γ value. This is because the d level of a heavier element is higher in energy and the corresponding d wavefunction with a stronger bonding is more extended. This is also true for elements in the same row in the periodic table where a heavier element has more d electrons [8]. An exception is in the VA series where the γ value of Nb is smaller than that of V possibly due to the rehybridization of Nb where Nb, whose d shell is less than half full, rehybridizes in the opposite direction, i.e., depletes the d_z^2 orbitals based on a charge density difference analysis [35–37].

γ values for sp metals except for Be are smaller than those for d metals due to the bond nature of s and p electrons, which are more mobile than the localized d electrons and therefore less energy is needed to break these bonds.

Table 1. S, Z_S and Z_B values for different surfaces and structures where S denotes the area of the two-dimensional unit cell; a and c are lattice constants. For A2, the CN of surface and bulk metals are divided into the nearest and the next-nearest bonds. CN is determined by equations (6)–(8). For A3 metals, an ideal c/a ratio (1.633) is assumed.

Structure	Surface	S	Z_S	Z_B
A1	(111)	$\sqrt{3}a^2/4$	9	12
	(100)	$a^2/2$	8	12
	(110)	$\sqrt{2}a^2/2$	6	12
A2	(110)	$\sqrt{2}a^2/2$	$Z_S = 6, Z_S' = 4$	$Z_B = 8, Z_B' = 6$
	(100)	a^2	$Z_S = 4, Z_S' = 4$	$Z_B = 8, Z_B' = 6$
	(111)	$\sqrt{3}a^2$	$Z_S = 2, Z_S' = 0$	$Z_B = 8, Z_B' = 6$
A3	(0001)	$\sqrt{3}a^2/2$	9	12
	($10\bar{1}0$)	$\sqrt{8/3}a^2$	16/3	12
A4	(110)	$\sqrt{2}a^2/5$	$Z_S = 3, Z_S' = 6$	$Z_B = 4, Z_B' = 12$
sc	(100)	a^2	$Z_S = 5, Z_S' = 8$	$Z_B = 6, Z_B' = 12$
	(110)	$\sqrt{2}a^2$	$Z_S = 4, Z_S' = 7$	$Z_B = 6, Z_B' = 12$

For A1 metals in table 2 save for Ca, Sr and Al, the mean-square root error σ between the predicted and the experimental results for the most close-packed (111) is about 7.5%. For Al, as the surface is present or CN decreases, the degree of covalent Al–Al bonding increases, or the nature of the bonding changes with reduced CN [40]. Since our formula neglects the case of bonding variation, the model prediction for Al deviates from the experimental results. The reason that there are deviations between the predicted γ values and the experimental results as well as the first-principles calculations for Ca and Sr is not clear.

For A3 metals, $\sigma \approx 10\%$ except Mg, Zn, Cd and Tl. For Cd and Tl, both our predictions and FCD calculations deviate evidently from the experimental results. In the case of Zn and Cd, c/a ratios (1.86 and 1.89) are larger than the ideal value of 1.633. Thus, the nearest CN values differ from the ideal condition, which should contribute the deviation of our prediction.

For sc metals, $\sigma = 2.6\%$ where Sb and Bi with the rhombohedral structure are assumed to have a slightly distorted sc structure [6] and their γ values are calculated in terms of the sc structure.

For A2 metals, $\sigma = 10\%$. Since the next-nearest CN is considered, A4 metals can also be determined based on the same equation. The smallest value of σ in all considered structures appears for A4 crystals, whose $\sigma = 1.4\%$. This result implies that the pure coherent bond does not change after a CN deduction.

Note that the temperature dependence of surface energy in our model is ignored although the experimental results listed in tables 2–4 are calculated at 0 K while most lattice constants cited are measured at room temperature. This temperature effect decreases the prediction accuracy of our model and may be partly responsible for the disagreement with other experimental and theoretical results.

4. Comparison between the above formula predictions and the first-principles calculations

In FCD calculations, there are often exceptions where the most close-packed surface does not have the lowest γ values or there exists a weak orientation dependence [6]. These physically unacceptable results are fully avoided in our calculation. In addition, the anisotropy in our formula is perfectly considered. $\gamma_{(100)}/\gamma_{(111)} \approx 1.16$ and $\gamma_{(110)}/\gamma_{(111)} \approx 1.27$ for A1 metals

Table 2. Comparison of surface energies of A1 metals among the predicted values γ based on equation (3), the FCD calculations γ' [6] and the experimental results γ'' [4, 5]. Note that the original E values in kJ mol^{-1} should be transformed to coherent energy per surface area in J m^{-2} by dividing by the Avogadro constant N_a and S. E and a are cited from [33] and [6, 34]. S and CN are come from table 1. The symbol *, which has the same meaning in tables 3 and 4, denotes that when the low-temperature equilibrium crystal structure has a lower symmetry than a close-packing phase at high temperature or under high pressure, the latter is utilized [6].

	E (kJ mol^{-1})	a (Å)	(hkl)	γ (J m^{-2})	γ' (J m^{-2})	γ'' (J m^{-2})
Cu	336	3.66	(111)	1.83	1.95	1.79, 1.83
			(100)	2.17	2.17	
			(110)	2.35	2.24	
Ag	284	4.18	(111)	1.20	1.17	1.25, 1.25
			(100)	1.40	1.20	
			(110)	1.51	1.24	
Au	368	4.20	(111)	1.52	1.28	1.51, 1.50
			(100)	1.80	1.63	
			(110)	1.94	1.70	
Ni	428	3.58	(111)	2.44	2.01	2.38, 2.45
			(100)	2.88	2.43	
			(110)	3.11	2.37	
Pd	376	3.85	(111)	1.85	1.92	2.00, 2.05
			(100)	2.15	2.33	
			(110)	2.35	2.23	
Pt	564	4.02	(111)	2.54	2.30	2.49, 2.48
			(100)	2.98	2.73	
			(110)	3.24	2.82	
Rh	554	3.87	(111)	2.70	2.47	2.66, 2.70
			(100)	3.15	2.80	
			(110)	3.41	2.90	
Ir	670	3.91	(111)	3.19	2.97	3.05, 3.00
			(100)	3.74	3.72	
			(110)	4.06	3.61	
Pb	196	5.11	(111)	0.55	0.32	0.59, 0.60
			(100)	0.64	0.38	
			(110)	0.70	0.45	
Al	327	4.05	(111)	1.45	1.20	1.14, 1.16
			(100)	1.68	1.35	
			(110)	1.84	1.27	
Ca	178	5.62	(111)	0.43	0.57	0.50, 0.49
			(100)	0.50	0.54	
			(110)	0.55	0.58	
Sr	166	6.17	(111)	0.33	0.43	0.42, 0.41
			(100)	0.39	0.41	
			(110)	0.43	0.43	
Mn*	282	3.53	(111)	1.65	3.10	1.54, 1.60
			(111)	0.90	0.87	
Ac	410	5.79	(100)	1.03	0.73	
			(110)	1.14	0.68	
			(111)	1.61	1.48	1.50
Th	598	5.19	(100)	1.85	1.47	
			(110)	2.36	1.45	

Table 3. Comparison of surface energies of A2, sc and A4 crystals among the predicted values γ based on equation (5), the FCD calculations γ' [6] and the experimental results γ'' [4, 5]. S and CN come from table 1.

	E (kJ mol^{-1})	a (Å)	(hkl)	γ (J m^{-2})	γ' (J m^{-2})	γ'' (J m^{-2})
Li	158	3.99	(110)	0.50	0.56	0.52, 0.53
			(100)	0.58	0.52	
			(111)	0.72	0.59	
Na	107	4.20	(110)	0.29	0.25	0.26, 0.26
			(100)	0.34	0.26	
			(111)	0.41	0.29	
K	90.1	5.30	(110)	0.16	0.14	0.13, 0.15
			(100)	0.18	0.14	
			(111)	0.23	0.15	
Rb	82.2	5.71	(110)	0.12	0.10	0.12, 0.11
			(100)	0.15	0.11	
			(111)	0.18	0.12	
Cs	77.6	6.26	(110)	0.10	0.08	0.10, 0.10
			(100)	0.12	0.09	
			(111)	0.14	0.09	
Ba	183	5.03	(110)	0.36	0.38	0.38, 0.37
			(100)	0.41	0.35	
			(111)	0.51	0.40	
Ra	160	5.37	(110)	0.27	0.30	
			(100)	0.32	0.29	
			(111)	0.40	0.32	
Eu	179	4.58	(110)	0.43	0.49	0.45, 0.45
			(100)	0.50	0.46	
			(111)	0.61	0.52	
V	512	3.02	(110)	2.74	3.26	2.62, 2.56
			(100)	3.26	3.03	
			(111)	4.04	3.54	
Cr*	395	2.85	(110)	2.39	3.51	2.35, 2.30
			(100)	2.83	3.98	
			(111)	3.50	3.89	
Fe	413	2.86	(110)	2.52	2.43	2.42, 2.48
			(100)	2.92	2.22	
			(111)	3.62	2.73	
Nb	730	3.76	(110)	2.58	2.69	2.66, 2.70
			(100)	2.99	2.86	
			(111)	3.72	3.05	
Mo	658	3.17	(110)	3.20	3.45	2.91, 3.00
			(100)	3.81	3.84	
			(111)	4.62	3.74	
Ta	782	3.35	(110)	3.40	3.08	2.90, 3.15
			(100)	4.05	3.10	
			(111)	5.01	3.46	
W	859	3.58	(110)	3.36	4.01	3.27, 3.68
			(100)	3.90	4.64	
			(111)	4.84	4.45	
Sb (sc*)	265	3.36	(100)	0.66	0.61	0.60, 0.54
			(110)	0.77	0.66	

Table 3. (Continued.)

	E (kJ mol^{-1})	a (Å)	(hkl)	γ (J m^{-2})	$\gamma\prime$ (J m^{-2})	$\gamma\prime\prime$ (J m^{-2})
Bi	210	3.26	(100)	0.55	0.54	0.49, 0.49
(sc*)			(110)	0.64	0.54	
Po	144	3.34	(100)	0.38	0.44	
(sc*)			(110)	0.44	0.37	
Si	446	7.71	(110)	1.06		1.14
(A4)						
Ge	372	8.10	(110)	0.80		0.88
(A4)						

as well as $\gamma_{(0001)}/\gamma_{(10\bar{1}0)} = 1.22$ for A3 metals, which show the agreement with the latest theoretical values of 1.15 and 1.22 [8, 27]. In addition, $\gamma_{(100)}/\gamma_{(110)} \approx 1.16$ for sc and A2 metals, which is especially comparable with 1.14 for monovalent sp metals based on the jellium model [39].

If the experimental results are taken as reference, 60% of our predicted γ values of the most close-packed surfaces of 52 elements shown in tables 2–4 have better agreements with the experimental ones than those of the FCD calculations do while 20% of the FCD calculations show the reverse. Note that the LDA method is used in our formula while the GGA method is used in FCD. Recently, it has been shown that both methods need to be corrected due to the neglect of surface electron self-interactions where GGA is worse than LDA [35–37]. This is surprising because GGA is generally considered to be the superior method for energetic calculations [6].

For the transition metals and noble metals, the formula works better than for others as the greatest contribution to bonding is from the s–d interaction and the orbitals of the latter localize, which is more like a pair interaction. According to tables 2–4, the predicted γ values of divalent sp metals have bad correspondence with the experimental results since the many-body (e.g. trimer) terms are here critical to understanding the cohesive energy. Thus, the used pair potentials may not be fully correct physically. It is possible that the background of our formula, namely the broken-bond model, is not universally applicable although the lattice constants used in equations (3) and (5) have a measuring error of about 2% [4, 20].

According to the first-principles calculations, the effect of relaxation on the calculated γ value of a particular crystalline facet may vary from 2 to 5% depending on the roughness [36, 38]. The semi-empirical results indicate further that the surface relaxation typically affects the anisotropy by less than 2% [13]. Surface relaxations for vicinal surfaces have been studied mainly using semi-empirical methods due to the complexity arising from the simultaneous relaxation of a large number of layers [8]. In our formula, the relaxation effect is simply considered by adding equation (2) to (1). According to tables 2–4, this measure leads to satisfactory results.

It should be noted that as a simple model without free parameters, the above formula supplies a new insight and another way for general estimation of surface energy of elements. This success is difficult to achieve for any first-principles calculation. Moreover, our model also supplies a basis for comparison and supplement for further theoretical and experimental considerations on γ values of elements.

5. Conclusion

In conclusion, a unified formula introduced by a modified broken-bond rule is utilized to predict surface energies of A1–A4 and sc crystals. At least for transition metals and noble metals, a

Table 4. Comparison of surface energies of A3 metals among the predicted values γ based on equation (3), the FCD calculations γ' [6] and the experimental results γ'' [4, 5]. S and CN are come from table 1. c/a ratios of Zn and Cd are cited from [6]. In FCD calculations the A3 structure has two $(10\bar{1}0)$ surfaces depending on the first interlayer distance d, $(10\bar{1}0)_A$ refers to the surface with $d_A = 0.29a$ while $(10\bar{1}0)_B$ denotes the surface with $d_B = 2d_A$. Here the results for $(10\bar{1}0)_A$ surface are present.

	E (kJ mol^{-1})	a (Å)	$(hkil)$	γ (J m^{-2})	γ' (J m^{-2})	γ'' (J m^{-2})
Be	320	2.22	(0001)	2.40	1.83	1.63, 2.70
			$(10\bar{1}0)$	2.88	2.13	
Mg	145	3.20	(0001)	0.53	0.79	0.79, 0.76
			$(10\bar{1}0)$	0.65	0.78	
Zn	130	2.68	(0001)	0.66	0.99	0.99, 0.99
		$(c/a = 1.86)$	$(10\bar{1}0)$	0.72		
Cd	112	3.06	(0001)	0.44	0.59	0.76, 0.74
		$(c/a = 1.89)$	$(10\bar{1}0)$	0.47		
Tl	182	3.71	(0001)	0.49	0.30	0.60, 0.58
			$(10\bar{1}0)$	0.60	0.35	
Sc	376	3.30	(0001)	1.25	1.83	1.28
			$(10\bar{1}0)$	1.53	1.53	
Ti	468	2.95	(0001)	1.96	2.63	1.99, 2.10
			$(10\bar{1}0)$	2.39	2.52	
Co	424	2.53	(0001)	2.42	2.78	2.52, 2.55
			$(10\bar{1}0)$	2.95	3.04	
Y	422	3.55	(0001)	1.22	1.51	1.13
			$(10\bar{1}0)$	1.49	1.24	
Zr	603	3.25	(0001)	2.08	2.26	1.91, 2.00
			$(10\bar{1}0)$	2.54	2.11	
Tc	661	2.74	(0001)	3.22	3.69	3.15
			$(10\bar{1}0)$	3.93	3.90	
Ru	650	2.72	(0001)	3.20	3.93	3.04, 3.05
			$(10\bar{1}0)$	3.90	4.24	
La*	431	3.87	(0001)	1.05	1.12	1.02
			$(10\bar{1}0)$	1.28	0.92	
Lu	428	3.51	(0001)	1.27	1.60	1.23
			$(10\bar{1}0)$	1.55	1.42	
Hf	621	3.20	(0001)	2.22	2.47	2.19, 2.15
			$(10\bar{1}0)$	2.71	2.31	
Re	775	2.76	(0001)	3.72	4.21	3.63, 3.60
			$(10\bar{1}0)$	4.54	4.63	
Os	788	2.75	(0001)	3.80	4.57	3.44, 3.45
			$(10\bar{1}0)$	4.64	5.02	

good correspondence among our formula, experimental results and other theoretical works is found.

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