

SURFACE ENERGY AND SURFACE STRESS OF DEFORMED METALS

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Abstract

In this work a model for computing the surface energy and surface stress of deformed metals were developed based on the structureless pseudopotential formalism. The developed models were tested by using them to compute the surface energy and surface stress of different classes of metals for different values of strain deformation. The results obtained revealed that deformation causes a reduction of surface energy and this reduction in surface energy is more pronounced in simple and alkaline metals. For surface stress of deformed metals, tensile stress is present in most metallic surfaces, although a few metals possess compressive stress on their surfaces. In the presence of deformation, the surface stress of some metals decreases. For Ti and Pt, deformation causes an increase in their surface stress, while deformation causes an increase in the surface stress of Mo and W causing the stress on their surfaces to change from compressive to tensile. But for Cr, Be and Al, the stress on their surfaces changes depending on the amount of deformation..

Keywords: Deformation, metals, stress, surface energy and structureless pseudopotential formalism.

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1. Introduction

Surface energy is one most important and fundamental electronic properties of metals that controls a wide range of phenomenon such as stress for brittle fracture, the rate of sintering and the growth rate during particle coarsening. The surface electronic properties of metals are greatly influenced by deformation and are often monitored by the measurement of the surface energy. Surface energy is the energy require to create unit area of new surface and can also be describe as the amount of work per unit area required to split an infinite crystal into two halves [1].

Surface stress is the solid state analogue of surface tension. Surface stress is essential where dynamical, structural and morphological issues are studied [2]. The surface stress originates from the nature of chemical bonding of atoms at the metallic surface. The atoms in the surface are bonded differently from the atoms in the interior of the metallic surface. Consequently, the atoms at the surface of an undeformed metal would have equilibrium inter atomic distance different from that of the interior atoms if the surface atoms were not constrained to remain structurally coherent with the underlying lattice [3]. Atoms at the surface and interior of metals changes during deformation along with their atomic distance depending on the metallic surface area that is subjected to different deformation. Surface stress play vital roles in surface construction and reconstruction, shape transition in nanoscale particles, surface alloying, surface diffusion epitaxial growth and self-assembled domain patterns [2].

Surface stress influence surface stability, defect formations, deformations and dynamics of metal surfaces. During deformation, the contact potential difference at the metal surface changes [4]. Consequently, a lot of efforts have been made to study surface energy and surface stress of deformed metals theoretically and experimentally. Kiejna, and Pogosov, [5] performed an experimental investigation on the effect of deformation on some electronic properties of metals by taking the direct measurement of deformed metal using Kelvin method. They observed that the contact potential

difference of the metals increase| when compressed and decreases when tensed. Monnier and Perdew [6] computed self – consistently the surface energy and its face dependence for some metals. The results obtained for seven of these nine metals were in good agreement with measured surface tension and the ionic pseudopotential of these metals gave a good account of the bulk binding energy. Marcus et al., [7] used the composite elastic model to calculate the surface stress obtained for the (001) face of Mo. The surface stress obtained for the (001) face of Mo was tensile. Kiejna, [8] calculated the surface energy of some simple metals using the structureless pseudopotential model. The results obtained were in good agreement with experimental values. Zang et al., [9] calculated the surface energy of bcc transition metals using the second nearest neighbor 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.

In this work, the surface energy and surface stress of deformed elemental metals consisting of monovalent, divalent, trivalent, noble and transition metals were computed using the structureless pseudopotential model modified for deformed metals. This will enable us test the strength of the structureless pseudopotential model in predicting the properties of deformed metals and this provide an insight into how the surface properties of metals varies with deformation. The metals used in this study were chosen based on the availability of experimental data, their industrial and technological applications, and availability of some physical constants of metals that is required for computation.

2.0 Theoretical Considerations

2.1 Surface Energy of Deformed Metal

Surface energy of metal is the energy required to create a new unit area [10]. For a metal under the action of a deforming force, the average electron density in such a metal as a function of deformation and is expressed as [4]

$$n = n_0 [1 - (1 - 2\nu)u_{xx}] + 0(u_{xx}^2) \quad (1)$$

where ν is the poisson ratio relating compression to elongation in the direction of applied deformation, u_{xx} is the strain and n_0 is the average electron density in the bulk of undeformed metal and is given by

$$n_0 = \frac{3}{4\pi r_s^3} \quad (2)$$

where r_s is the electron density parameter of undeformed metal. For a deformed metal, the average electron density parameter of the metal is

$$r_{su} = r_s [1 + (1 - 2\nu)u_{xx}]^{\frac{1}{3}} \quad (3)$$

The energy functional of a stabilized jellium is [8]

$$E[n, n_+] = E_j[n, n_+] + (E_m + W_R) \int d^3r n_+(r) + \langle \delta v \rangle_{ws} \int d^3r \theta(r) [n(r) - n_+(r)] \quad (4)$$

where E_j is the jellium total energy functional given as

$$E_j = T_s[n] + E_{xc}[n] + \frac{1}{2} \int d^3r \phi([n, n_+], r) [n(r) - n_+(r)] \quad (5)$$

where $T_s[n]$ 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 (4) does not contribute to the surface energy of deformed metal since it is purely a bulk property of the metal. The electrostatic potential is expressed as

$$\phi([n, n_+], r) = \int \frac{n(r') - n_+(r')}{|r - r'|} dr' \quad (6)$$

For a Wigner-Seitz cell of radius r_0 , the electrostatic potential of the uniformly charged sphere is

$$V(r) = \frac{eQ(r)}{r} + e \int_r^{r_0} n \frac{d\Omega}{r} \quad (7)$$

where $Q(r) = \frac{4\pi r^3}{3}$ is the charge inside the sphere of radius r , n is the average electron density and

Ω is the volume. Hence

$$V(r) = \begin{cases} \frac{ze}{r_0} \left(\frac{3}{2} - \frac{r^2}{2r_0} \right) & r < r_0 \\ \frac{ze}{r} & r > r_0 \end{cases} \quad (8)$$

The average potential over the Wigner-Seitz cell of radius r_0 is

$$\langle \delta_{wu} \rangle_{av} = \frac{1}{z} \int_0^{r_0} dr 4\pi r^2 n(w(r)) + V(r) \quad (9)$$

but

$$w(r) = 2\pi n r_c^2 \quad (10)$$

hence

$$\frac{1}{z} \int_0^{r_0} dr 4\pi r^2 n\left(\frac{z}{r}\right) = \frac{3z}{2r_0} \quad (11)$$

so

$$\langle \delta_{wu} \rangle_{av} = 2\pi n r_c^2 - \frac{3z}{2r_0} \quad (12)$$

The surface energy of the stabilized jellium can be decomposed into

$$\sigma_{sj} = \sigma_{jell} + \langle \delta_{wu} \rangle_{av} \int_0^{\infty} dx [n(x) - n] \quad (13)$$

where σ_{jell} is the standard jellium surface energy function. The jellium surface energy is made up of the kinetic, electrostatic and the exchange-correlation energy functional given as

$$\sigma_{kinetic} = \frac{1}{2\pi^3} \int_0^{k_f} dk' k^3 \left(n_k - \frac{\pi}{4} \right) - \int_{-\infty}^{\infty} dx n(x) [V_{eff}(x) - V_{eff}(\infty)] \quad (14)$$

where n_k is the phase shift, V_{eff} is the effective potential. The electrostatic energy functional is given as

$$\sigma_{electrostatic} = \frac{1}{2} \int_{-\infty}^{\infty} dx \phi(x) [n(x) - n_+(x)] \quad (15)$$

while the exchange-correlation component is

$$\sigma_{exchange\ corr} = \int_{-\infty}^{\infty} dx n(x) [E_{xc}(n(x)) - E_{xc}(n_{av})] \quad (16)$$

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

For a given r_c the average stabilization potential can be obtained from

$$\langle \delta_{wu} \rangle_{av} = \bar{n} \frac{d}{dn} (E_m + \bar{w}_R) \quad (17)$$

The stabilization condition of the stabilized jellium is

$$\frac{d}{dn} (E_s(\bar{n}) + E_{xc}(\bar{n}) + E_m + \bar{w}_R) = 0 \quad (18)$$

but

$$\langle \delta_{wu} \rangle_{av} = \bar{n} \frac{d}{dn} [t_s + E_{xc}(\bar{n})] \quad (19)$$

where t_s is the kinetic energy and E_{xc} is exchange correlation energy. So

$$\sigma_{ps} = \langle \delta_{wu} \rangle_{av} \int_{-\infty}^0 dx [n(x) - n_+(x)] \quad (20)$$

Substituting equation (19) into (20) we have

$$\sigma_{ps} = \bar{n} \frac{d}{dn} [t_s + E_{xc}(\bar{n})] \int_{-\infty}^0 dx [n(x) - n_+(x)] \quad (21)$$

The surface energy of deformed metal can be decomposed as

$$\sigma = \sigma_s + \sigma_{es} + \sigma_{xc} + \sigma_{ps} \quad (22)$$

where σ_s is the kinetic energy, σ_{es} is the electrostatic energy, σ_{xc} is the exchange- correlation energy and σ_{ps} is the pseudopotential surface energy term

The kinetic, electrostatic and exchange correlation contributions were computed using the parameterized expressions of Brajczewska et al., [11], while the pseudopotential contribution was computed using equation (21) using the kinetic, exchange, and correlation energies in the low density limit of the density functional theory approximation.

2.2 Surface Stress of Deformed Metal

The change in the total energy of a system during the change in the surface elastic strain tensor of the deformation tensor is given by [12] as

$$\delta E = \int \sum_{ij} \sigma_{ij}(r) \delta \varepsilon_{ij} dr \quad (23)$$

where $\sigma_{ij}(r)$ is the stress tensor at a point r. considering the geometry of the metal and assuming periodicity in x and y directions, then the change in energy as

$$\delta E = A \int_{-d/2}^{d/2} \sum_{ij} \tau_{ij}(z) \delta \varepsilon_{ij} dz \quad (24)$$

where d is the thickness of the metal slab and $\tau_{ij}(z)$ are the components of the metal slab stress tensor given as

$$\tau_{ij}(z) = \frac{1}{A} \int \sigma_{ij}(r) dx dy \quad (25)$$

where $\tau_{ij}(z)$ is

$$\tau_{ij}(z) = \int \left[\tau_{ij}(z) - \tau_{ij}^{(b)} \right] dz \quad (26)$$

and $\tau_{ij}^{(b)}$ is the stress tensor in the bulk region. The surface stress tensor in equation (24) can be separated into two parts as

$$\delta E = 2\delta E^S + \delta E^{(b)} = 2A \sum_{ij} \tau_{ij}^{(s)} + Ad \sum_{ij} \tau_{ij}^{(b)} \delta \varepsilon_{ij} \quad (27)$$

The factor of two comes from the two surfaces of the metal slab. From equation (27),

$$\delta E^{(s)} = \frac{1}{2} [\delta E - \delta E^{(b)}] = A \sum_{ij} \tau_{ij}^{(s)} \delta \varepsilon_{ij} \quad (28)$$

and

$$\tau_{ij}^{(s)} = \frac{1}{A} \frac{\partial E^{(s)}}{\partial \varepsilon_{ij}} \quad (29)$$

Note that $E^{(s)} = A\sigma$, where σ is the surface energy. So we can write

$$\tau_{ij}^{(s)} = \frac{1}{A} \frac{\partial A\sigma}{\partial \varepsilon_{ij}} = \sigma \delta_{ij} + \frac{\partial \sigma}{\partial \varepsilon_{ij}} \quad (30)$$

where $\partial \sigma / \partial \varepsilon_{ij}$ is the residual stress, δ_{ij} is the kronecker delta function, i, j denote the directions in the surface plane surface.

Based on the work of Needs and Godfrey [13], the surface stress can be written as

$$\tau(n) = \sigma - n_o \frac{d\sigma}{dn_o} \quad (31)$$

The second term in the right hand of equation (17) is the strain derivative of the surface energy which in terms of r_{su} is given [13] as

$$-n_o \frac{d\sigma}{dn_o} = \frac{r_{su}}{3} \frac{d\sigma}{dr_{su}} \quad (32)$$

Hence, for a deformed metal,

$$\tau = \sigma + \frac{r_{su}}{3} \frac{d\sigma}{dr_{su}} \quad (33)$$

where σ is the surface energy, r_{su} is the electron density parameter of a deformed metal.

In this work, the surface energy and surface stress of deformed metals were computed using equation (22) and equation (33) and how deformation affects these surface properties of metals are studied..

3 Results and Discussion

3.1 Surface Energy of Deformed Metal

Fig. 1 shows the variation of surface energy with electron gas parameter of some elemental metals consisting of alkaline, earth alkaline, transition and noble metals. Figure 3.1 revealed that the surface energy decreases with increase in the electron gas parameter as metals in the high-density region has high surface energy. As shown in Figure 3.1, for the electron gas parameter between $1.70 \leq r_s \leq 2.65$ a.u the surface energy of metals are very close but for $r_s \geq 3$ a.u it observed that there is a clear difference between the surface energy of the metals as we move from one metals to another. The decrease in surface energy as the electron gas parameter increases may be due to the interaction between the electrons on the surface and those in the bulk which is affected by the electronic concentration of the metals. The results of the surface energy shown in Fig.1 based on structureless pseudopotential model were quite in good agreement with the results obtained by Skriver and Rosengaard [14] that made *ab initio* study of the surface energy of 40 elemental metals by means of Green's – function technique based on linear – muffin –tin – orbitals method within the tight –binding and atomic sphere approximation. In Fig. 1, as the electron gas parameter increases, the surface energy decreases. This seems to suggest that surface energy of metals depends on the electronic concentration of metals as metals in the high density limit have high surface energy. Furthermore, metals in the low – density limit have low values of the surface energy.

Fig. 2 shows the variation of surface energy with deformation for some elemental metals. As shown in the figure, surface energy of metals decreases with an increase in deformation, while metals in the high

density region has high surface energy and metals in the low density region has low surface energy just like the case of undeformed metals shown in Fig. 1. Table 1 revealed that Molybdenum and Tungsten has the highest surface energy when all the metals investigated were subjected to deformation while Fig. 2 revealed that potassium has the lowest surface energy when it is subjected to deformation. The trend exhibited by Fig. 2 and Table 1 revealed that the surface energy of metals is greatly affected by deformation also, the results obtained shows that as the strain is increased, the surface energy of the metals decrease. This may be due to the fact that the applied strain causes an increase in atomic spacing in metals, reduces electron-electron interactions with a consequential decrease in surface energy of metals.

3.2 Surface Stress of Deformed Metal

Figure 3 shows the variation of surface stress with electron gas parameter for some elemental metals consisting of alkaline, alkaline-earth, transition and noble metals. Fig. 3 revealed that the surface stress of metals increases from the high-density limit, get to a maximum at about $r_s = 2.5$ a.u and decreases towards the low-density limit. The figure further revealed that the computed surface stress for some metals are positive showing that tensile stress is present on the metallic surfaces. This is in agreement with results obtained using other models. [3,15]. The resulting positive stress may be due to the positive strain derivative that prevails on the surfaces of the metals [1]. The results obtained in Fig. 3 revealed that for $r_s < 2$ a.u, Be, Ti, Cr, Mo, and W that lies in this density range have compressive stress on their surfaces. This may be due to the inward bonding of the electrons on their surfaces or a negative strain derivative. The metallic surfaces may have a curvature on the surfaces as a result of the inward bonding of the electrons at the surface. Also, Fig.3 reveals that the surface stress of metals increases from the high density limit, gets to a maximum at about $r_s = 2.5$ a.u and decreases towards the low-density limit.

Fig. 4 shows the variation of surface stress of deformed metals with strain for some elemental metals. The figure reveals that the surface stress on potassium surface is not affected significantly by strain. But for Cu, Ag, and Fe, strain causes a decrease in the surface stress of these metals. This reveals that the applied strain or deformation causes changes in the bonding of the electron on the surface of these metals and also causes a change in the strain derivative of these metals. Also, the figure reveals that the surface stress of metals in the high- density limit is high while the surface stress of metals in the low density limit is low. This seems to suggest that the surface stress of metals depends on the electronic concentration of the metals.

Table 2 shows the variation of the surface stress of different metals with strain. The table clearly reveals that deformation affects the surface stress of metals. For K, Cu, Ag, Mg, Fe, Zn, Cd, Bi, Sn, Pb, Au and Ta, the stress on their surfaces decreases with increase in strain. But for Cr, Be, and Al, the surface stress increases with increase in strain, gets to a maximum value and starts to decrease. This shows that surface stress of metals is affected by some other structural properties. The surface stress of Ti and Pt increases with an increase in deformation.

Also, Table 2 reveals that strain changes the surface stress of Mo and W from compressive to tensile depending on the amount of the applied strain. For Mo and W as the applied strain is increased, the compressive stress on their surfaces reduces, but for strain ≥ 1.5 , the stress on their surfaces becomes tensile. The above observation reveals that surface stress of metals depends on some properties such as nature of the surface, nature of the electrons on the surface, the type of bonding between electrons on the surface. The stress at the surface may be affected by the internal stress in the metals.

The results obtained in this work for the surface energy and surface stress of metals compares favourably with the results of Osiele and Olubosede, [16], In the work of Osiele and Olubosede,[16] the stress of all the metals they computed were tensile and they did not investigate the effect of strain

on the surface stress of metals. The result of the surface energy of metals obtained in this work compares very well with that of Lang and Kohn,[10], The surface stress of metals computed in this work compares favourably well with the results of Marcus et al.,[7] and Kollar et al.,[12] for undeformed metals. Furthermore, the results obtained in this work for the surface energy and surface stress of deformed metals are in good agreement with the theoretical predictions of Pogosov et al.,[4], and that of Kiejna and Pogosov [1].

4 Conclusion

The surface energy and surface stress of some deformed metals were successfully computed using the stabilized jellium model. The results obtained revealed that the surface energy of metals decreases with an increase in deformation. In the high density region the surface energy and surface stress of deformed metals is high while it is small for metals in the low density region. The stress on a metal surface could be tensile or compressive depending on the electron gas parameter of the metal. Deformation causes a change in the surface stress of metals. For some metals, deformation causes a reduction in the stress on their surfaces. For some, deformation causes an increase in the surface stress of the metals and deformation can cause the stress to change from compressive to tensile.

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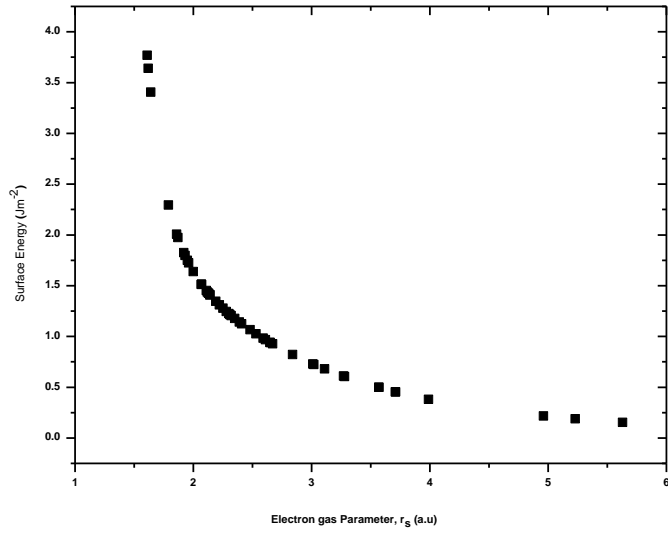


Fig 1: Variation of surface energy with electron gas parameter for some metals

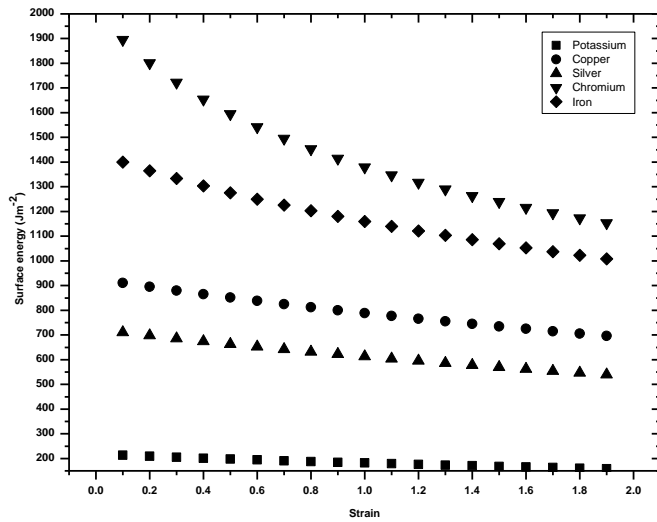


Fig 2: Variation of surface energy with deformation for some metals.

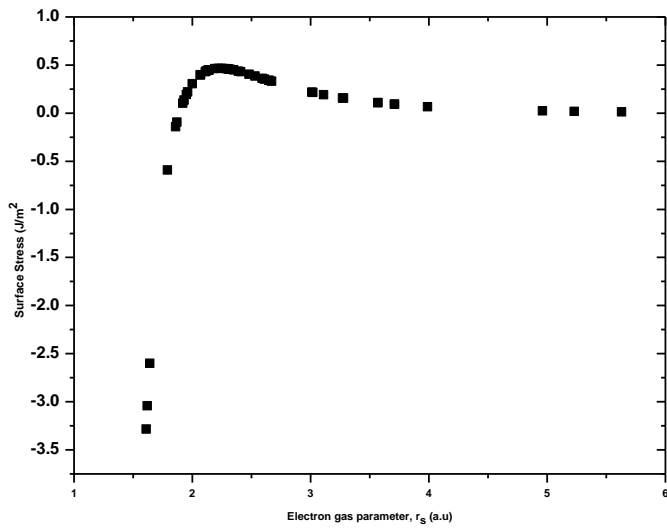


Fig. 3: Variation of surface stress with electron gas parameter for some metals.

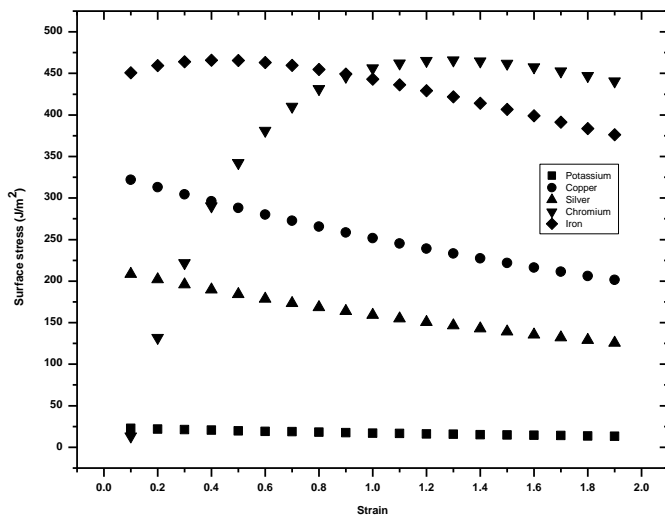


Fig. 4: Variation of surface stress with deformation for some metals.

Table 1: Surface energy of deformed metals

Metal	r_s (a.u.)	Strain								
		0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	208	201	194	188	182	176	171	166	161
Cu	2.67	895	866	838	813	789	766	745	725	706
Ag	3.02	698	675	653	632	613	595	578	562	547
Be	1.87	1680	1499	1372	1275	1196	1130	1073	1022	978
Mg	2.65	906	874	845	817	792	768	746	725	705
Cr	1.86	1801	1654	1542	1453	1380	1318	1264	1216	1173
Fe	2.12	1365	1303	1250	1202	1159	1121	1086	1053	1022
Ni	2.07	1437	1372	1316	1267	1223	1184	1147	1114	1083
Zn	2.31	1167	1124	1085	1049	1016	985	956	929	904
Cd	2.59	936	894	856	822	790	761	734	709	685
Al	2.07	1444	1385	1333	1287	1246	1208	1174	1142	1112
Bi	2.25	1226	1180	1139	1102	1067	1035	1005	977	951
Ti	1.92	1714	1624	1550	1486	1431	1382	1338	1298	1262
Y	2.61	907	854	807	766	728	695	664	636	611
Sn	2.22	1258	1210	1168	1129	1094	1061	1031	1003	976
Pb	2.30	1205	1185	1166	1148	1131	1114	1098	1083	1068
Mo	1.61	3327	2988	2721	2508	2334	2191	2072	1971	1884
W	1.62	3144	2781	2508	2297	2130	1996	1886	1794	1716
Au	2.39	1119	1097	1079	1060	1042	1025	1008	992	976
Pt	2.00	1584	1535	1492	1452	1416	1383	1352	1323	1297
Ta	2.84	789	760	734	709	686	664	644	625	607

Table 2: Surface stress of deformed metals

Metals	r_s (a.u.)	strain							
		0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	20.47	19.20	18.05	17.00	16.04	15.17	14.37	13.63
Cu	2.67	296	280	265	252	239	227	216	206
Ag	3.02	190	179	169	159	151	143	136	129
Be	1.87	408	458	465	453	433	409	384	360
Mg	2.65	301	284	268	254	241	228	217	206
Cr	1.86	290	381	431	456	465	465	458	447
Fe	2.12	466	463	455	443	429	414	399	384
Ni	2.07	458	465	465	459	450	439	426	413
Zn	2.31	430	414	397	380	364	348	333	318
Cd	2.59	312	291	271	253	236	221	208	195

Al	2.07	455	464	466	463	456	447	437	426
Bi	2.25	449	436	421	406	390	375	360	345
Ti	1.92	317	376	415	440	456	463	466	464
Y	2.61	289	262	239	218	200	184	170	158
Sn	2.22	457	445	432	418	403	388	373	359
Pb	2.30	450	445	439	433	426	420	413	406
Mo	1.61	-1816	-1330	-952	-656	-423	-238	-90.7	27.34
W	1.62	-1438	-952	-594	-327	-127	25.30	140.7	228.5
Au	2.39	420	411	402	394	385	376	368	359
Pt	2.00	386	412	436	446	455	462	465	466
Ta	2.84	236	221	208	196	184	174	165	156