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Research Article

Vibrational Internal Energy And Helmholtz Free Energy Of Metals

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ABSTRACT

This article revealed an interesting issue on vibrational internal energy and Helmholtz free energy of metals. The relationship existing between the lateral strain and axial strain was taking into consideration during computation. Vibrational internal energy and Helmholtz free energy of metals was computed and studied based on the theory of free electron approximation using the knowledge of thermodynamic potentials. Computed and theoretically obtained experimental valueof vibrational internal energy and Helmholtz free energy of metals agreed quite well with each other.Vibrational internal energy of metals increases as temperature increasesdue to change in atomic configuration mode and valence electron exchange between ions in metals.Increase in vibrational internal energy of metals as strain increases can be caused by weak electron cohesion and uncertainties regarding the behavior of valence electrons, atomic size, atomic configuration and bonding interaction between the electron in metals. Result obtained for free energy of metals is negative throughout which indicate that there is a better binding between electron in metals. Free energy of metals decreases as temperature increases due to reduction in atomic interaction and bond strength between the interacting electron in metals. Free energy of metals decreases as strain increases.

Keywords: Vibrational energy, free energy, strain/deformation, tensile strength, Fermi energy, free electron approximation, thermodynamic potential.

INTRODUCTION

Metals occupy a special position in the study of solids,metals play a prominent role in theory of solids and has proved to be one of great fundamental states of matter (Kakani and Kakani, 2004). Metals are excellent conductors of heat and electricity, metals are ductile and malleable (Kittel, 1976). The challenge of accounting for metallic features and properties providestarting impetus to modern theory of solids (Animalu, 1977).With thermodynamics, one is able to control the structure of solid material without knowing the atomic details of the crystals(Rogalski and Palmer, 2000). The knowledge of both classical thermodynamics and statistical mechanics represents a powerful combination in the study of crystalsstructures (Kakani and Kakani, 2004).Free energy is an extensive property of solid and its magnitude depends on the amount of substance in thermodynamic state (Ashcroft and Mermin, 1976). Free energy has dimensions of energy and its value is determined by state of the system. Free energy is used to determine how system change and work produce (Madelung, 1995). Thermodynamic potentials H, F and G defined in terms of U and TS has thermal properties of free electron gas regarded as temperature independent at normal temperature range (Pillai, 2010).Metals are deformed when subject to an applied mechanical stress. Stress is a measure of applied mechanical force normalized to take into account cross sectional area. Strain represents the amount of deformation induced by stress (Kakani and Kakani, 2004). Poisson's ratio is an important elastic constant and its value is different for different materials. Poisson's ratio describesthe relationship existing between lateral strain and axial strain (Elliott, 1997).Before now, a lot of theoretical model has been developed by researchers to study and investigatethe characteristic properties of solids in a qualitative and quantitative way and brilliant successes have been recorded.Tyson and Miller, (1977), derived a semi-theoretical equation which expresses solid-vapor surface free energy as a function of liquid surface tension and solid-liquid interfacial free energy. He obtained a solid-liquid energy which gives accurate estimate of solid surface energy at melting temperature for large number of elements with dependable liquid surface tension. This result agrees quite well with available experimental values when compared. Ahmed (2018), investigate the surface free energy of metallic nanoparticles in bulk material using a theoretical model that involves specific term for computing cohesive energy of nanoparticle. The results obtained revealed that surface energy is appropriate for spherical nanoparticle with realistic shape of nanoparticle. The surface energy of copper, silver, gold, platinum, tungsten, molybdenum, tantalum, palladium and alkali metallic nanoparticles is prominent in nanoscale size, and it decreases with reduction of nanoparticle size. A decrease in surface energy is found by moving from bulk to atom. This result is consistent with other reported data. Aziz and Patrice (2006), calculate some thermodynamic properties using molecular simulation. Result obtained agree quite well with experimental thermodynamic binding properties. A novel method for computing entropy changes from a molecular dynamics' simulation is demonstrated and expression for free energy, entropy and enthalpy in ensemble was establish using Free Energy Perturbation (FEP) formalism. The change in thermodynamic properties association of inorganic cations with a macrocycle of biological interest is illustrated. Lynden-Bell et. al. (1993), Investigated the variation in Landau free energy while melting platinum at different temperatures using computer simulation with model potential. He applied a biasing potential in a Monte Carlo simulation with umbrella sampling technique. The results obtained from Landau free energy curves gives accurate values of the difference in free energies between solid and liquid phases, thermodynamic melting point and metastability limit of crystalline phase. There was no evidence for nucleation of a metastable body-centered-cubic phase due to existence of local icosahedral order in metallic liquid phase. Adesakin et. al (2019) develop a model for computing current density, drift velocity and electron mobility of metals based on free electron theory. The results obtained for variation of this properties of metals with electron density parameter are in agreement with experimental value. Current density of metals reduces as deformation rises while the drift velocity and electron mobility rise as deformation increases. In this study, vibrational internal energy and Helmholtz free energy of metalswas computed and studied based on theory of free electron theory approximation using the knowledge of thermodynamic potential.

Computational methods

The total vibrational internal energy which is the internal energy is obtain by summing over all normal modes. Considering a continuous distribution of frequencies $N(\omega)$ since the normal frequencies lie close together to replace the sum by integral

$$U = \int_0^{\omega_{max}} E(\omega)N(\omega)d\omega = \int_0^{\omega_{max}} \frac{\hbar\omega}{exp\left(\hbar\omega/_{k_BT}\right)-1} N(\omega)d\omega \tag{1}$$

where $E(\omega)$ is the mean energy expressed in the form

$$\langle E_k\rangle = \sum_{n_k=0}^{\infty} E_k p(n_k) = \frac{\sum_{n_k=0}^{\infty} E_k exp\left(-E_k/_{k_BT}\right)}{\sum_{n_k=0}^{\infty} exp\left(-E_k/_{k_BT}\right)} = \frac{\sum_{n_k=0}^{\infty} n_k\hbar\omega_k exp\left(-n_k\hbar\omega_k/_{k_BT}\right)}{\sum_{n_k=0}^{\infty} exp\left(-n_k\hbar\omega_k/_{k_BT}\right)} + \frac{1}{2}\hbar\omega_k \tag{2}$$

setting $x = exp\left(-\hbar\omega_k/_{k_BT}\right)$in equation (2) the equation becomes

$$\langle E_k\rangle = \left[\frac{\sum_{n_k=0}^{\infty} n_k x^{n_k}}{\sum_{n_k=0}^{\infty} x^{n_k}} + \frac{1}{2}\right]\hbar\omega_k = \left[\frac{x\sum_{n_k=0}^{\infty} n_k x^{n_k-1}}{\sum_{n_k=0}^{\infty} x^{n_k}} + \frac{1}{2}\right]\hbar\omega_k = \left(\frac{x}{1-x} + \frac{1}{2}\right)\hbar\omega_k =$$

$$\left(\frac{1}{exp\left({\hbar\omega_k}/{k_BT}\right)-1}+\frac{1}{2}\right)\hbar\omega_k = E(\omega_k) \tag{3}$$

where use has been made of the identity

$$\sum_{n_k=0}^{\infty} n_k x^{n_k-1} = \frac{d}{dx}\sum_{n_k=0}^{\infty} x^{n_k} = \frac{d}{dx}\left(\frac{1}{1-x}\right) = \frac{1}{(1-x)^2} \tag{4}$$

and $N(\omega)d\omega$ is the number of oscillators with frequencies in the range between ω and $\omega + d\omega$, ω_{max} is the highest frequency of any normal mode. The lattice heat capacity is express as

$$c_v = \left(\frac{\partial U}{\partial T}\right)_v = \int_0^{\omega_{max}} k_B\left(\frac{\hbar\omega}{k_BT}\right)^2 \frac{exp\left({\hbar\omega}/{k_BT}\right)}{\left(exp\left({\hbar\omega}/{k_BT}\right)-1\right)^2} N(\omega)d\omega = \frac{\pi^2}{2}NK_B\left(\frac{T}{T_F}\right) \tag{5}$$

It is common practice to drop the zero-point energy in equation (1) as it has no contribution to the heat capacity. The frequency distribution function for linear monatomic lattice with a cut-off frequency ω_{max} is obtained as

$$N(\omega) = \frac{{2N}/{\pi}}{\left(\omega_{max}^2-\omega^2\right)^{1/2}} \tag{6}$$

Substituting equation (6) into equation (1) we obtain

$$U = \frac{2N\hbar}{\pi}\int_0^{\omega_{max}} \frac{\omega d\omega}{\left(exp\left({\hbar\omega}/{k_BT}\right)-1\right)\left(\omega_{max}^2-\omega^2\right)^{1/2}} \tag{7}$$

At low temperatures $(\hbar\omega \ll k_BT)$, assuming the highest frequency modes are effectively frozen, such that ${\omega_{max}}/{\omega} \gg 1$, hence

$$U = \frac{2N\hbar}{\pi}\int_0^{\omega_{max}} \frac{d\omega}{\left(\exp\left({\hbar\omega}/{k_BT}\right)-1\right)\left[\left({\omega_{max}}/{\omega}\right)^2-1\right]^{1/2}} = \frac{2N\hbar}{\pi\omega_{max}}\int_0^{\omega_{max}} \frac{\omega d\omega}{\left(exp\left({\hbar\omega}/{k_BT}\right)-1\right)} \tag{8}$$

Setting $x = {\hbar\omega}/{k_BT}$ and $\theta_D = {\hbar\omega_{max}}/{k_BT}$, then

$$U = \frac{2Nk_BT^2}{\pi\theta_D}\int_0^{{\theta_D}/{T}} \frac{xdx}{exp(x)-1} = \frac{\pi Nk_B}{3\theta_D}T^2 \tag{9}$$

where T is temperature, k_B is the Boltzmann constant, N is the number of particles and θ_D is Debye temperature obtained as

$$\theta_D = \frac{\hbar\gamma}{K_B}\left(6\pi^2\frac{N}{V}\right)^{\frac{1}{3}} = \frac{\hbar\gamma}{K_B}\left(6\pi^2\eta\right)^{\frac{1}{3}} \tag{10}$$

where, γ is the average sound velocity and the ratio $\frac{N}{V} = \eta$ is the electronic concentration.

The entropy of the free electron gas is obtained using the relation

$$S = \int_0^T \frac{Cv}{T}dT \tag{11}$$

Substituting the electronic heat capacity in equation (5) into equation (11), the entropy of the free electron gas is obtainedas

$$S = \int_0^T \frac{1}{T}\frac{\pi^2}{2} N k_B \left(\frac{T}{T_F}\right) dT = \frac{\pi^2}{2} \mathrm{N} K_B \left(\frac{T}{T_F}\right) \tag{12}$$

Evaluating the integral in equation (12) we have

$$S = \frac{\pi^2}{2} \mathrm{N} K_B \left(\frac{T}{T_F}\right) \tag{13}$$

Multiplying equation (13) by T, hence

$$\mathrm{TS} = \frac{\pi^2}{2} N K_B T_F \left(\frac{T}{T_F}\right)^2 \tag{14}$$

The Helmholtz free energy is given by

$$F = U - TS \tag{15}$$

Putting equation (9) and (14) into equation (15) we obtain

$$F = \frac{\pi N k_B}{3\theta_D} T^2 - \frac{\pi^2}{2} N K_B T_F \left(\frac{T}{T_F}\right)^2 \qquad = \pi N k_B \ T^2 \left(\frac{1}{3\theta_D} - \frac{\pi}{2T_F}\right) \tag{16}$$

where N is electron density of state,k_B is Boltzmann constant, T is temperatureand T_F is Fermi temperature. In this article, vibrational internal energyand Helmholtz free energy of metals were computed using equation (9)and (16) and how vibrational internal energy and Helmholtz free energy of metals changes with linearly applied strain is examined.

RESULTS AND DISCUSSION

Figure 1 shows variation of vibrational internal energy with electron density parameter for metals from different groups and periods. Both computed and theoretically obtained experimental value agree quite well with each other. Figure 1 revealed that vibrational internal energy of metals depends on ratio of valence electrons to their number of atoms as most of the metals whose vibrational internal energy were computed have their mobile electron concentrated in high density region than low density region. The trend demonstrated by metals in figure 1 also indicates that the higher the electronic structure in metal the higher the vibrational internal energy. Figure 2 shows variation of vibrational internal energy at different temperature with electron density parameter. In figure 2, vibrational internal energy of metals rises as temperature increases. This could be due to change in atomic configuration mode and valence electron exchange between ions in metals.Figure 3 shows variation of vibrational internal energy with strain for metals belonging to different elemental group and period.In figure 3, vibrational internal energy of metals rises as strain increases. This increase is caused by increase in lattice vibration,and electron disorder in metals. In figure 3, increase in vibrational internal energy of metals as strain increases can be caused by weak electron cohesion and uncertainties regarding the behavior of valence electrons, atomic size, atomic configuration and bonding interaction between the electron in metals.Figure 4 shows variation of free energy with electron density parameters for metals belonging to different groups and periods. There is agreement between computed and theoretically obtained experimental value. Result obtained for free energy of metals is negative throughout which seems to suggest a favorable and spontaneous electron reaction. Negative value of free energy of metals obtained in this work also indicate that there is a better binding between electron in metals andalso indicate that metals have free mobile electron in them which liberates energy that can be harnessed to do usefulwork. Result obtained in figure 4 revealed that free energy of metals decreases as electron density parameter of metals increases.

This shows that the higher the density of valence electron in metal the higher the free energy of metals and the lower the density of valence electron in metal the lower the free energy of metals. Furthermore, the trend display by metals in figure 4 also revealed that free energy of metals is highly dependent on electronic concentration. Figure 5 shows variation of free energy of metals at different temperature with electron density parameter for monovalent, divalent, trivalent and polyvalent metals. The trend display by metals in figure 5 revealed that free energy of metals decreases as temperature increases. This seems to suggest that as temperature increases the atomic interaction and bond strength between interacting electron in metals reduces which their-by forces the free energy of metals to decrease as temperature increases. Figure 6 shows variation of free energy with strain for metals belonging to different groups and periods. Also, reduction if free energy as strain increases can be due to reduction in atomic packing and electron affinity in metals. In figure 6, strain seems not to be having much effect on free energy of Fe, Cr, Ag and Cu as these could be due to their electronicnature, ionization energyand crystalline structure.The trend display by free energy in figure 4, 5 and 6 define Helmholtz free energy as F=U-TS which means that F can only decrease and can only move to lower and lower values.

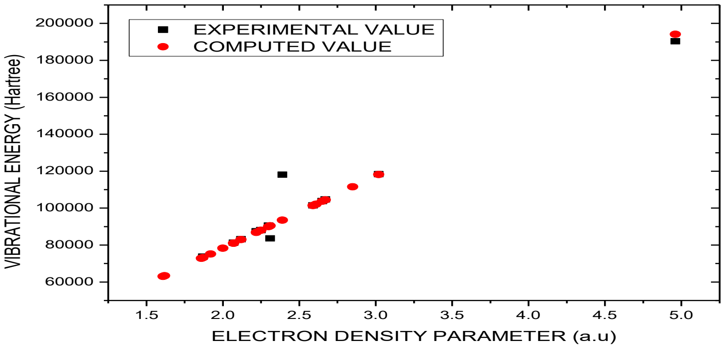

Figure 1: Variationof Vibrational Energywith Electron Density Parameterfor some Metals

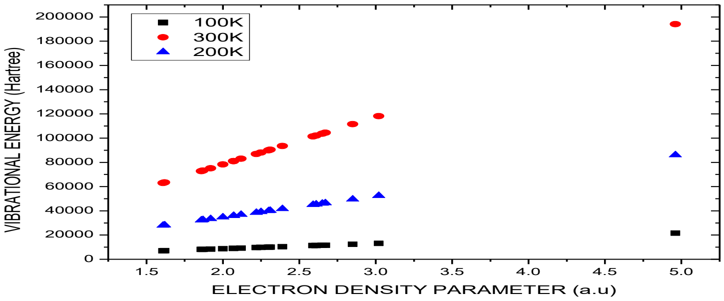

Figure 2: Variationof Vibrational Energyat Different Temperaturewith Electron Density Parameterfor some Metals

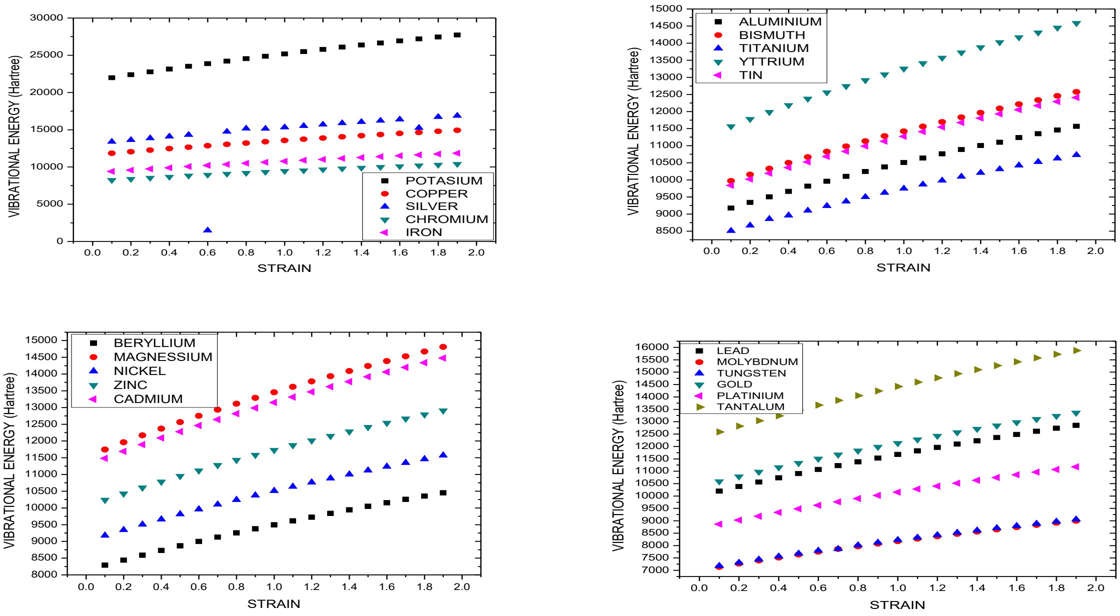

Figure 3: Variationof Vibrational Energywith Strainforsome Metals

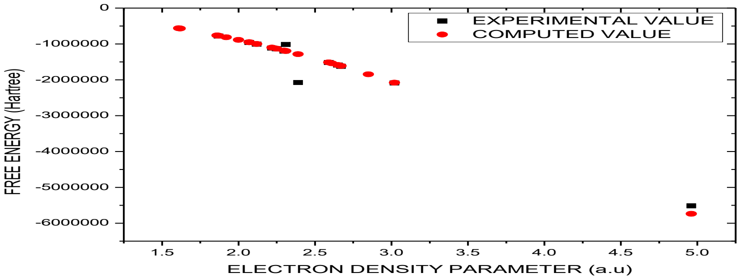

Figure 4: Variationof Free Energywith Electron Density Parameterforsome Metals

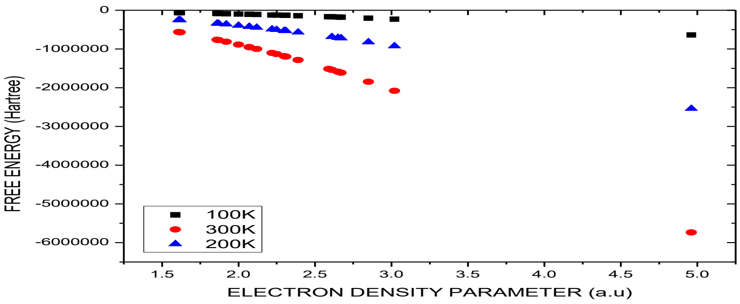

Figure 5: Variationof Free Energyat Different Temperaturewith Electron Density Parameterfor some Metals

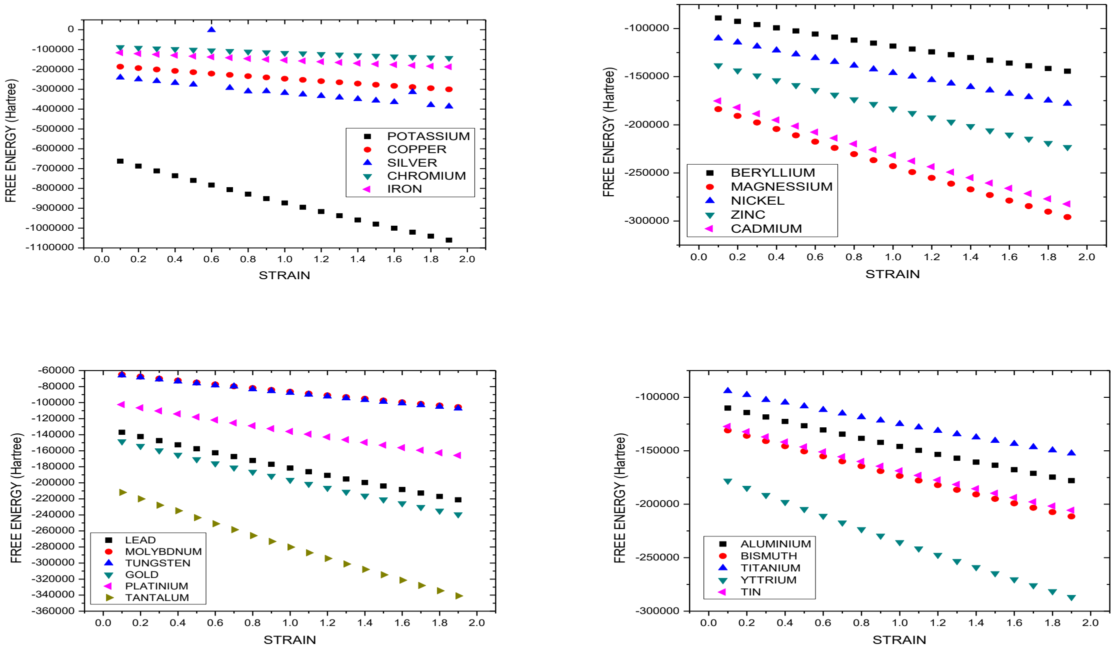

Figure 6: VariationofFree Energywith Strainforsome Metals

Table 1: Vibrational Energy and Helmholtz Free Energy of unstrained Metals.

Metals	Electron Density Parameter r_s(a.u)	Exp. Vibrational Energy (Hartree)	Computed Vibrational Energy (Hartree	Exp. Helmholtz Free Energy (Hartree)	Computed Helmholtz Free Energy (Hartree)
K	4.96	190341	194087	-5.513E06	-5.736E06
Cu	2.67	104753	104478	-1.623E06	-1.614E06
Ag	3.02	118378	118174	-2.088E06	-2.080E06
Be	1.87	73699.8	73173.9	-781467	-769834
Mg	2.65	103789	103696	-1.592E06	-1.589E06
Cr	1.86	-	72782.5	-	-761234
Fe	2.12	83181.0	82956.5	-1.006E06	-1.001E06
Ni	2.07	-	81000.0	-	-951951
Zn	2.31	83560.8	90391.3	-1.016E06	-1.196E06
Cd	2.59	101454	101348	-519E06	-1.516E06
Al	2.07	81261.3	81000.0	-958363	-951951
Bi	2.25	88078.4	88043.5	-1.133E06	-1.132E06

Ti	1.92	-	75130.4	-	-813555
Y	2.61	-	102130	-	-1.540E06
Sn	2.22	87503.1	86869.6	-1.118E06	-1.101E06
Pb	2.30	90538.3	90000.0	-1.200E06	-1.185E06
Mo	1.61	-	63000.0	-	-561907
W	1.62	-	63391.3	-	-569302
Au	2.39	118056	93521.7	-2.076E06	-1.283E06
Pt	2.00	-	78260.9	-	-886016
Ta	2.84	-	111522	-	-1.846E06

Table 2: Vibrational Energy of Deformed Metals

		Strain								
Metals	r_s (a.u)	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	22387.0	23151.7	23868.3	24543.7	25183.3	25791.6	26372.0	26927.7	27460.9
Cu	2.67	12051.0	12462.7	12848.5	13212.0	13556.3	13883.8	14196.3	14495.3	14782.4
Ag	3.02	13635.1	14096.4	1489.26	15161.3	15333.4	15703.7	16057.2	16395.5	16720.1
Be	1.87	8440.26	8728.57	8998.74	9253.39	9494.52	9723.87	9942.70	10152.2	10353.2
Mg	2.65	11960.8	12369.3	12752.2	13113.1	13454.8	13779.8	14089.9	14386.7	14671.7
Cr	1.86	8395.13	8681.87	8950.61	9203.87	9443.74	9671.87	9889.52	10097.9	10297.8
Fe	2.12	9568.65	9895.48	10201.8	10490.4	10763.9	11023.6	11271.9	11509.4	11737.3
Ni	2.07	9342.96	9661.87	9961.17	10243.0	10510.0	10763.8	11006.1	11238.0	11460.5
Zn	2.31	10426.2	10782.3	11116.1	11430.7	11728.5	12011.8	12282.1	12540.9	12789.3
Cd	2.59	11690.0	12089.3	12463.5	12816.2	13150.2	13467.8	13770.9	14061.0	14339.5
Al	2.07	9342.96	9662.09	9961.17	10243.0	10510.0	10763.8	11006.1	11238.0	11460.5
Bi	2.25	10155.4	10502.3	10827.3	11133.7	11423.9	11696.3	11963.1	12215.0	12457.0
Ti	1.92	8665.91	8962.13	9239.35	9500.78	9748.39	9983.83	10208.5	10423.7	10630.0
Y	2.61	11780.3	12182.7	12559.7	12915.1	13251.7	13571.8	13877.2	14169.6	14450.2

Sn	2.22	10020.0	10362.3	10683.0	10985.3	11271.6	11543.8	11803.6	12052.3	12291.0
Pb	2.30	10381.1	10735.7	11068.0	11381.2	11677.8	11959.8	12229.0	12486.6	12733.9
Mo	1.61	7266.74	7514.96	7747.57	7966.83	8174.44	8371.87	8560.26	8740.61	8913.74
W	1.62	7311.87	7561.65	7795.70	8016.30	8225.22	8423.87	8613.43	8794.91	8969.09
Au	2.39	10787.3	11155.8	11501.0	11826.5	12134.7	12427.8	12707.5	12975.2	13232.2
Pt	2.00	9027.00	9335.35	9624.30	9896.65	10154.6	10399.8	10633.9	10857.9	11073.0
Ta	2.84	12818.3	13234.5	13666.5	14053.3	14419.5	14767.8	15100.1	15418.3	15723.6

Table 3: Helmholtz Free Energy of Deformed Metals

		Strain								
Metals	r_s (a.u)	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	-687668	-736238	-783258	-828905	-873328	-916646	-958960	-1.0E+06	-1.04E+06
Cu	2.67	-193718	-207603	-221051	-234111	-246824	-259226	-271345	-283201	-294822
Ag	3.02	-249780	-267441	-1656.53	-310520	-317781	-333695	-349245	-364461	-379368
Be	1.87	-92501.2	-99225.9	-105741	-112072	-118236	-124251	-130130	-135884	-141524
Mg	2.65	-190737	-204412	-217656	-230519	-243041	-255254	-267189	-278868	-290312
Cr	1.86	-91469.8	-98120.7	-104566	-110826	-116924	-122874	-128689	-134380	-139958
Fe	2.12	-120164	-128850	-137265	-145439	-153399	-161157	-168752	-176179	-183458
Ni	2.07	-114342	-122610	-130632	-138419	-146001	-153398	-160627	-167703	-174636
Zn	2.31	-143600	-153945	-163965	-173699	-183175	-192420	-201453	-210295	-218959
Cd	2.59	-181935	-194988	-207630	-219909	-231862	-243522	-254915	-266065	-276991
Al	2.07	-114342	-122616	-130632	-138419	-146001	-153398	-160627	-167703	-174636
Bi	2.25	-135973	-145780	-155277	-164504	-173487	-182139	-190815	-199190	-207409
Ti	1.92	-97744.5	-104846	-111718	-118398	-124903	-131250	-137453	-143528	-149476
Y	2.61	-184846	-198105	-210946	-223417	-235560	-247402	-258974	-270299	-281396
Sn	2.22	-132239	-141780	-151023	-160001	-168741	-177269	-185603	-193760	-201752
Pb	2.30	-142314	-152568	-162501	-172149	-181543	-190706	-199660	-208424	-217012

Mo	1.61	-67559.1	-72509.4	-77306.8	-81969.3	-86509.5	-90940.5	-95271.6	-99511.9	-103669
W	1.62	-68446.2	-73460.2	-78318.6	-83040.2	-87638.7	-92125.9	-96512.2	-100807	-105016
Au	2.39	-154090	-165178	-175915	-186347	-196502	-206408	-216087	-225561	-234845
Pt	2.00	-106435	-114148	-121621	-128881	-135950	-142847	-149588	-156186	-162652
Ta	2.84	-219986	-234929	-250963	-265764	-280171	-294225	-307956	-321393	-334558

CONCLUSION

In summary, this work clearly demonstrates the behavior of metallic vibrational internal energy and Helmholtz free energy as a function of electron density parameter and linearly applied strain/deformation. This study is based on theory of free electron approximation.Result obtained agree quite well with theoretically obtained experimental value.Vibrational internal energy of metals depends on electronic concentration and statistical structure factor. Vibrational internal energy of metals increases as temperature and strain/deformation increases. Vibrational internal energy of metals depends on ratio of valence electrons to their number of atoms. Free energy of metals is negative throughout which seems to suggest a favorable and spontaneous electron reaction. Free energy of metals decreases as temperature and strain/deformation increases. Reduction of free energy as strain increases can be due to reduction in atomic packing and electron affinity in metals.

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