



## MEAN FREE PATH AND WAVELENGTH OF ELECTRON AT FERMI LEVEL OF METALS

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### Abstract

Mean free path and wavelength of electron at Fermi level for different groups and periods of metals were computed and studied based on the theory of free electron formalism using the knowledge of Fermi gas. Result obtained for the wavelength of electron at Fermi level is in good agreement with theoretical experimental value. This prove the validity of the theory of free electron formalism in theoretical predictions of some properties of metals. Result obtain in this work shows that mean free path of metal depend on number of valence electron, electronic concentration and collision frequency. Mean free path of metals decreases as strain (deformation) increases due to an increase in electron radius. Wavelength of electron at Fermi level reduces as the experimental value of Fermi energy of metals increases. Wavelength of electron at Fermi level increases as strain increases due to an increase in the internal degree of freedom. [E. Adesakin, F.O. Ogunlana T.H. Akande, O.G.Edema, J.O. Chukwu, O. O. Olusola , O.D. Afe, O.A. Fasiku, Agbetuyi Oluranti Adegoke and Faruq Oyediran. **MEAN FREE PATH AND WAVELENGTH OF ELECTRON AT FERMI LEVEL OF METALS.** *Nat Sci* 2024,22(7):6-14]. ISSN 1545-0740 (print); ISSN 2375-7167 (online). <http://www.sciencepub.net/nature> 02. doi:[10.7537/marsnsj220724.02](https://doi.org/10.7537/marsnsj220724.02).

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### 1.0 Introduction

Solids are classified based on their specific geometrical, mechanical and electrical properties. These classification helps to recognize the origin of their unique properties and to invent new solid with specific useful properties (Chih-Tang, 1991). Metals is an array of positive ions held together in a cloud of free electrons with their valence electrons moving freely. These electrons move within the metal due to electrostatic attraction between the positive ion cores (Puri and Babbar, 2008). Electrons are responsible for conduction of electricity through metals. This conduction electron move in a uniform electrostatics field and their potential energy remains constant by neglecting the existence of ion cores (Puri and Babbar, 2008). Mean free path is an average distance which an electron covers in its wavelike pattern without any reflection or deflection (Busch and Schade, 1976) and can also be describe as the average distance traveled by a moving particle between successive impacts or collisions which modify its direction, energy and other particle properties (Efthimios, 2003). Fermi wavelength is the de Broglie wavelength of electrons at the Fermi energy (Animalu, 1977). Metals are deformed when subject to an applied mechanical stress which change its shapes and sizes (Kittel, 1976). Stress is a measure of an applied

mechanical force normalized to take into account cross sectional area while strain represents the amount of deformation induced by stress (Kakani and Kakani, 2004). Before now, different theoretical and experimental research work has been performed by experimentalist and theorist to study some properties of metals using different computational and experimental techniques. Jennings (1988) presented the values of mean free path at different temperature for dry and moist air using an expression that minimizes the dependence on physical constants for mean free path. Result obtained agree quite well with the result of Cunningham slip correction factor when compared. Sooraj et. al (2013) determined the mean free path of rarefied gases using Molecular Dynamics simulations. The simulations are carried out on isothermal argon gas (Lennard-Jones fluid) over a range of rarefaction levels under various confinements (unbounded gas, parallel reflective wall and explicit solid platinum wall bounded gas) in a nanoscale domain. These studies provide insight to the transport phenomena of rarefied gases through nanochannels with potential in microscale and nanoscale heat transfer applications. Seunghwan (2019) use Monte Carlo (MC) simulation data to estimate the average mean-free-path length of multicomponent hydrocarbon molecules in an organic nanochannel base

on equilibrium distribution of gas molecule. The results obtain show that the smaller the channel the denser the gas mixture due to nanoconfinement effects. The mean-free-path lengths of the confined molecules is also computed using the trajectories of the molecules displaced over time in the equilibrium molecular dynamics (MD) simulation. Qixin and Zhivong (2014) studies the characteristics of gas molecular mean free path in nanopores using molecular dynamics simulation. The results obtain indicate that mean free path of all molecules in nanopores depend on the radius of the nanopore and interaction strength. The molecular mean free path varies with the molecule's distance from the center of the nanopore. The least value of the mean free path occurs at the wall surface of the nanopore. The radial gas molecular mean free path is much smaller than the mean free path including all molecular collisions occurring in three directions. Results obtain indicate that when gas is confined in nanopores the gas molecule density does not affect the gas molecular mean free path in the same way as it does for the gas in unbounded space. Nishanth et. al. (2010) derive an effective molecular mean free path model that allows the mean free path to vary close to bounding surfaces. This model is compared with molecular dynamics simulation data and other classical mean free path models of gas transport properties related to the mean free path through kinetic theory. Result obtained is compared with that of conventional hydrodynamic models, solutions of the Boltzmann equation and experimental data. It was found that probability distribution function describes better the mean free paths of dilute gas molecules in a confined system. Adesakin et. al. (2020) used a theoretical model approach to compute magnetic moment of metals based on free electron theory. The result obtained agree quite well with experimental value, this suggest that free electron theory is useful for theoretical prediction of some properties of metals. The results obtained shows that magnetic moment of metals depends on spin and orbital configuration. Magnetic field influence magnetic moment of metals due to rotation of magnetic dipole and that magnetic field in metals is weakened by induced magnetization. Magnetic moment of metals subjected to deformation decreases as strain increases. Magnetic moment of metals is determined by ratio of valence electrons to their number of atoms. Magnetic moment of all metals computed is negative, this is due to spin intrinsic properties and negative electric charge possess by electrons in metal. Adesakin et. al. (2012) develop a model for computing correlation, binding and cohesive energy of deformed and undeformed metals based on structureless pseudopotential formalism. Results obtained showed that correlation energy increases with increase in electron density parameter. An increase in deformation was found to cause corresponding increase in the correlation energy. Deformation causes a decrease

in the binding energy of metals and it does not cause a significant change in the cohesive energy of metals. Adesakin et. al. (2018) develop a model for computing relaxation time, Fermi velocity and Fermi temperature of deformed metals based on free electron theory. The result obtained shows qualitative agreement between the experimental and computed values of Fermi velocity, Fermi temperature and relaxation time of metals when compared. The Fermi velocity, Fermi temperature and relaxation time of all the metals subjected to different deformation decreases as deformation increases. This suggest that as deformation increases the collision frequency, inter-atomic spacing between the interacting electron decreases which forces the relaxation time, Fermi velocity and Fermi temperature to decrease as deformation increases.

## 2.0 Computational methods

A more accurate calculation of the electronic properties of metals is obtained from Schrodinger equation for N-particle wave function of all N electrons in metals

$$\psi(r_1s_1, r_2s_2, \dots \dots r_Ns_N)$$

$$H\psi = \sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \nabla_i^2 \psi - Ze^2 \sum_R \frac{1}{|r_i - R|} \psi \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} \psi = E\psi$$
(1)

where the negative potential energy term is the attractive electrostatic of bare nuclei fixed at points R of Bravais lattice and the last term is the interactions of the electrons with each other. The proper choice of the potential U(r) in the one-electron Schrodinger equation is

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + U(r)\psi(r) = \epsilon\psi(r)$$
(2)

where U(r) is the potentials of ions given as

$$U^{ion}(r) = -Ze^2 \sum_R \frac{1}{|r - R|}$$
(3)

By treating the remaining electrons as a smooth distribution of negative charge with charge density  $\rho$ , the potential energy of the given electron in their field is

$$U^{el}(r) = -e \int dr' \rho(r') \frac{1}{|r - r'|}$$
(4)

The contribution of an electron in the level  $\psi_i$  to the charge density is

$$\rho_i(r) = -e |\psi_i(r)|^2$$
(5)

The total charge density is

$$\rho(r) = -e \sum_i |\psi_i(r)|^2$$
(6)

and the sum extends over all occupied one electron levels in metal.

Substituting equation (6) into equation (4) and letting  $U = U^{ion} + U^{el}$  gives the one-electron equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(r) + U^{ion}(r)\psi_i(r) + \left[e^2\sum_j\int dr'|\psi_j(r')|^2\frac{1}{|r-r'|}\right]\psi_i(r) = \varepsilon_i\psi_i(r) \quad (7)$$

where the potential of the ions is precisely canceled by  $U^{ion} + U^{el} = 0$ , only the exchange term survives and is easily evaluated by writing the coulomb interaction in terms of its Fourier transform

$$\frac{e^2}{|r-r'|} = 4\pi e^2\frac{1}{V}\sum_q\frac{1}{q^2}e^{iq\cdot(r-r')} \rightarrow 4\pi e^2\int\frac{dq}{(2\pi)^3}\frac{1}{q^2}e^{iq\cdot(r-r')} \quad (8)$$

$$\text{Then } \varepsilon(k) = \frac{\hbar^2 k^2}{2m} - \frac{1}{V}\sum_{k' < k_F} \frac{4\pi e^2}{|k-k'|^2} = \frac{\hbar^2 k^2}{2m} - \int\frac{dk'}{(2\pi)^3}\frac{4\pi e^2}{|k-k'|^2} = \frac{\hbar^2 k^2}{2m} - \frac{2e^2}{\pi}k_F F\left(\frac{k}{k_F}\right) \quad (9)$$

$$\text{and } F(x) = \frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right| \quad (10)$$

equation (9) is the energy of the one electron level with wave vector  $k$ .

The contribution of interaction to the total energy of  $N$ -electron is the sum of this correction over all  $k < k_F$ .

$$E = 2\sum_{k < k_F} \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{\pi} \sum_{k < k_F} \left[1 + \frac{k_F^2 - k^2}{2kk_F} \ln\left|\frac{k_F + k}{k_F - k}\right|\right] \quad (11)$$

To find the velocity distribution for electrons in metals, consider a small volume element of  $k$ -space about a point  $k$  of volume  $dk$ . Allowing for two-fold spin degeneracy, the number of one-electron levels in this volume element is

$$N = \left(\frac{V}{4\pi^3}\right) dk \quad (12)$$

The probability of each level being occupied is  $f(\varepsilon(k))$  and the total number of electrons in  $k$ -space volume is

$$N = \frac{V}{4\pi^3} f(\varepsilon(k)) dk \quad (13)$$

where  $\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$  and the velocity of free electron with wave vector  $k$  is

$$V = \frac{\hbar k}{m} \quad (14)$$

The number of electrons in an element of volume  $dv$  about  $v$  is the same as the number in an element of volume  $dk = \left(\frac{m}{\hbar}\right)^3 dv$  about  $k = \frac{mV}{\hbar}$ .

Consequently, the total number of electrons per unit volume of real space in a velocity space element of volume  $dv$  about  $v$  is

$$N = f(v)dv \quad (15)$$

$$\text{where } f(v) = \frac{\left(\frac{m}{\hbar}\right)^3}{4\pi^3} \frac{1}{\exp\left[\frac{(1/2)mv^2 - \mu}{k_B T}\right] + 1} \quad (16)$$

the Fermi energy  $E_F$  is defined as

$$E_F = \frac{\hbar^2 k_F^2}{2m} \quad (17)$$

Fermi energy at absolute zero is equals the chemical potential  $\mu$  defined as the change in energy of a thermodynamic electronic system of  $N$  particles when one extra electron is added to it

$$\mu = E(N+1) - E(N) \quad (18)$$

The temperature variation of Fermi energy become

$$E_F(T) = E_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{E_F}\right)^2\right] \quad (19)$$

Expressing the Fermi characteristics in terms of electron density parameters  $r_s$ , the wavelength of electron at Fermi level and mean free path is

$$\lambda_F = 2\pi \left(\frac{4}{9\pi}\right)^{1/3} r_s = \frac{2\pi}{k_F} \quad (20)$$

and

$$\gamma = \frac{m_e}{ne^2\rho} \sqrt{2E_F} \quad (21)$$

where  $k_F$  is the Fermi wave-vector,  $m_e$  is the mass of electron,  $n$  is the electronic concentration,  $e$  is the electronic charge and  $\rho$  is the electrical resistivity. In this article, free electron theory approximation is used to compute the wavelength of electron at Fermi level and mean free path of metals using equation (20) and (21) and how wavelength of electron at Fermi level and mean free path of metals varies with linearly applied strain is investigated.

### 3.0 Result and Discussion

Figure 1 shows the plot of mean free path as a function of electron density parameter for different groups and periods of metals. Figure 1 revealed that mean free path of metals increases as the electron density parameter increases. This suggest that mean free path of metal depend on number of valence electron and electronic concentration. The trend demonstrated by metals in

figure 1 also revealed that mean free path of metals depend on collision frequency as the electron in metals whose mean free path were computed is more concentrated in the region of high-density limit than low density limit. Another factor that may be responsible for the increase in mean free path of metals in figure 1 may be due to an increase in the distance between the electrons in metal. Furthermore, the trend display by metals in figure 1 seems to suggest that the lower the number of electron per unit volume in metals the lower the mean free path of electron in metal and the higher the number of electron per unit volume in metals the higher the mean free path of electron in the metal. Figure 2 shows the plot of mean free path as a function of strain for different groups and periods of metals. Figure 2 revealed that mean free path of metals decreases as strain (deformation) increases. This may be due to reduction in electron strength in metals. The trend display by metals in figure 2 may also be due to weak electron localization that forces the mean free path of metals to decrease as strain increases. Figure 3 shows the plot of wavelength of electron at Fermi level as a function of experimental Fermi energy of metals. Figure 3 revealed that wavelength of electron at Fermi level reduces as the experimental Fermi energy of metals increases, with metals in the region of high- density limit having high value of wavelength of electron at Fermi level than metals in the region of low- density limit. This may be due to the fact that wavelength of electron at Fermi level depend highly on valence electron and effective distance between the electron in metals. In figure 3 there is a good agreement between the computed and experimental value of wavelength of electron at Fermi level. The experimental value of wavelength of electron at Fermi level is theoretically obtained by directly substituting the experimental value of Fermi energy obtained from solid state Physics by Charles Kittel, 1976 into the model used for computation. Figure 4 shows the plot of wavelength of electron at Fermi level as a function electron density parameter for metals from different groups and periods. Figure 4 revealed that there is a rapid linear increase in the wavelength of electron at Fermi level of metals from

the region of high-density limit to low density limit. The electron in metals are more concentrated in the region of high-density limit than low density limit. These suggest that wavelength of electron at Fermi level depend highly on effective distance between electron and number of valence electron per atom in metals. In figure 4, the computed and experimental value of wavelength of electron at Fermi level agree quite well with each other. The trend display by metals in figure 3 and 4 indicate that wavelength is inversely related to frequency and as well validate free electron theory formalism as a useful tool that can be relied upon in theoretical prediction of some properties of metals. Figure 5 shows the plot of wavelength of electron at Fermi level as a function of strain for metals from different groups and periods. Figure 5 revealed that wavelength of electron at Fermi level increases as strain increases. This may be due to an increase in the internal degree of freedom and the dynamics of electron near the Fermi level. Another factor that may be responsible for the increase in the wavelength of electron at Fermi level as strain increases is the increase in the energy of carrier electron, electron-electron scattering and phase randomizing of electron in metals. In conclusion, the trend demonstrated by metals in figure 5 indicates that wavelength of electron at Fermi level is highly influence by strain (deformation).

#### **Conclusion**

The mean free path and wavelength of electron at Fermi level has been evaluated by using the theory of free electron formalism. We obtain a good agreement between computed and experimental value of wavelength of electron at Fermi level. Mean free path of metals increases as the electron density parameter increases because of the increase in the electron inter-atomic distance. Mean free path of metals decreases as strain increases due some factors the it depends upon that is highly affected by deformation. Wavelength of electron at Fermi level depend highly on the effective distance between the electron in metals and the valence electron. wavelength of electron at Fermi level increases as strain increases due to an increase in the internal degree of freedom and the dynamics of electron near the Fermi level.

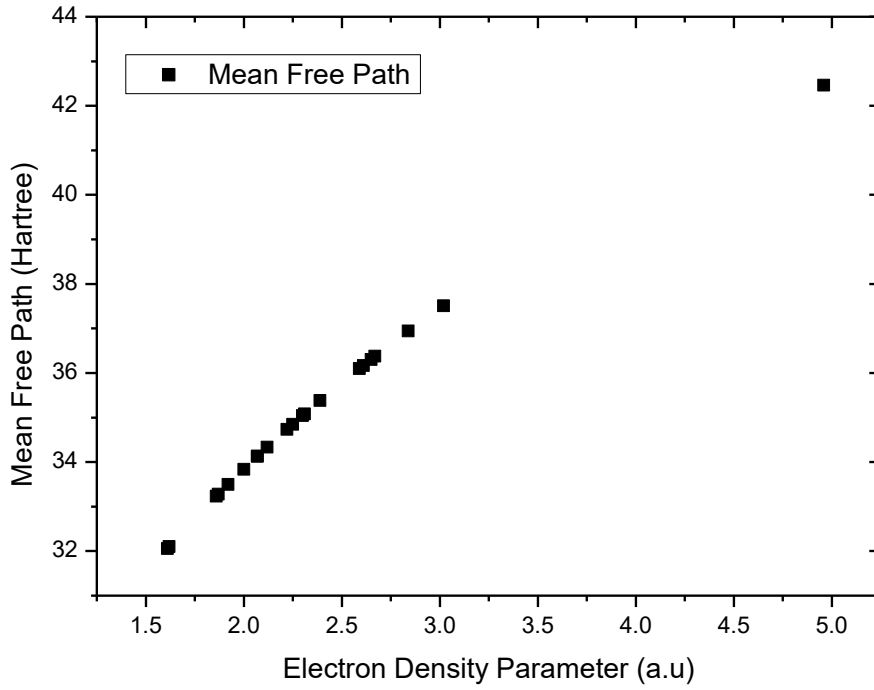


Figure 1: Mean Free Path as a function of Electron Density Parameter of Metal

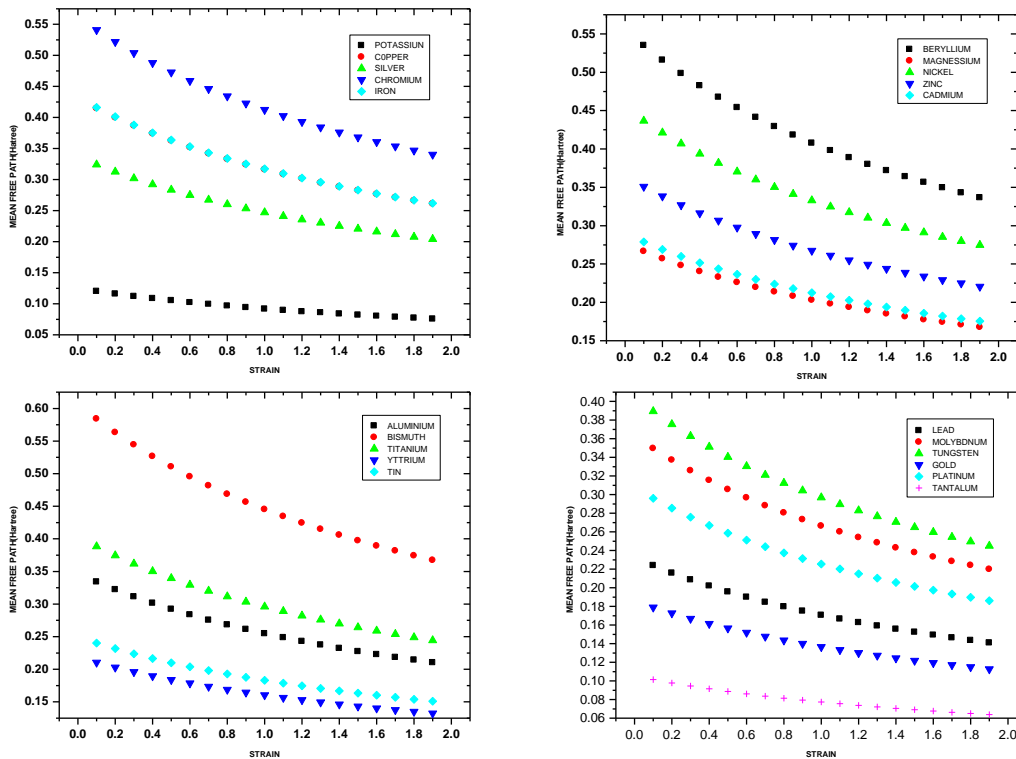


Figure 2: Mean Free Path as a function of Strain for Metals

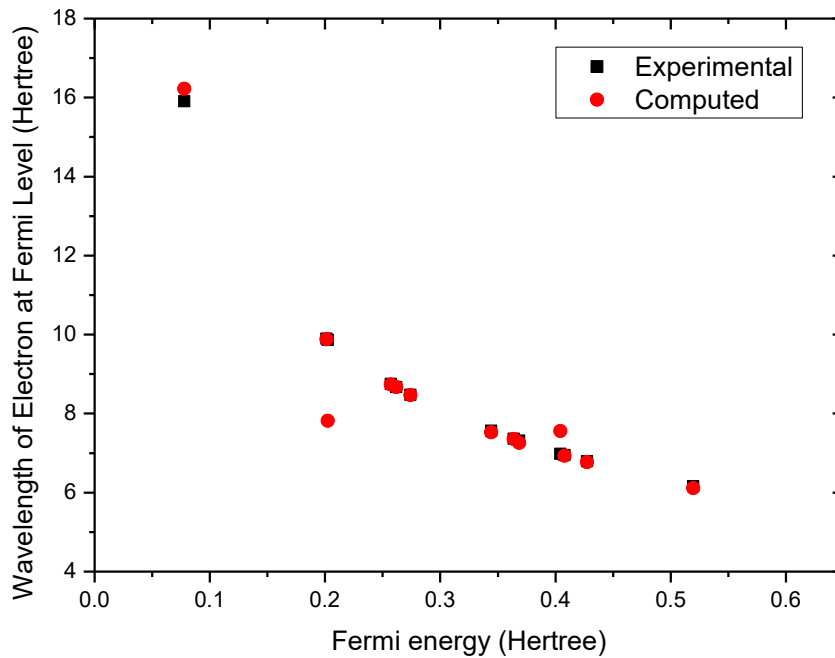


Figure 3: Wavelength of Electron at Fermi Level as a function of Experimental Fermi Energy of Metals

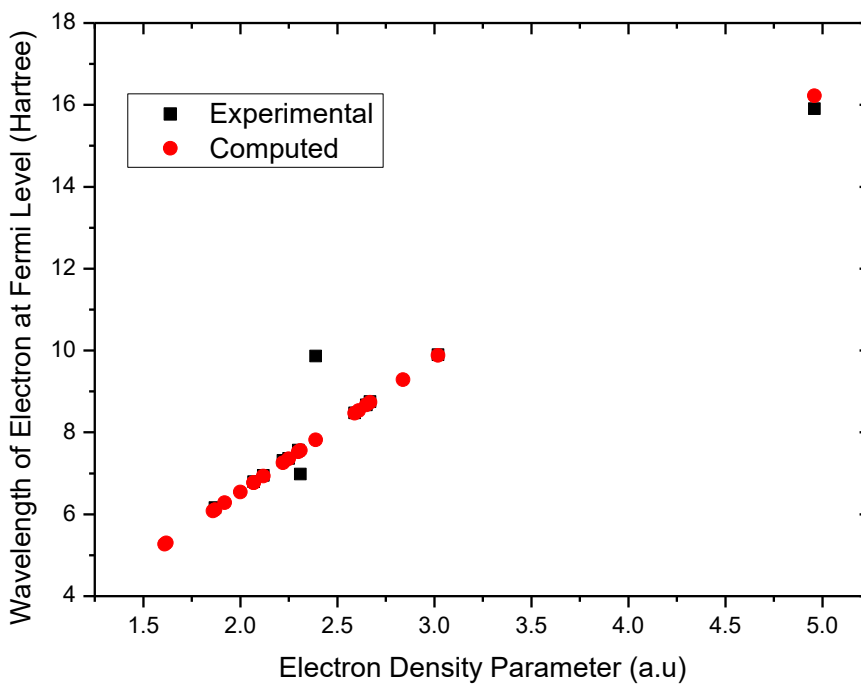


Figure 4: Wavelength of Electron at Fermi Level as a Function of Electron Density Parameter of Metals

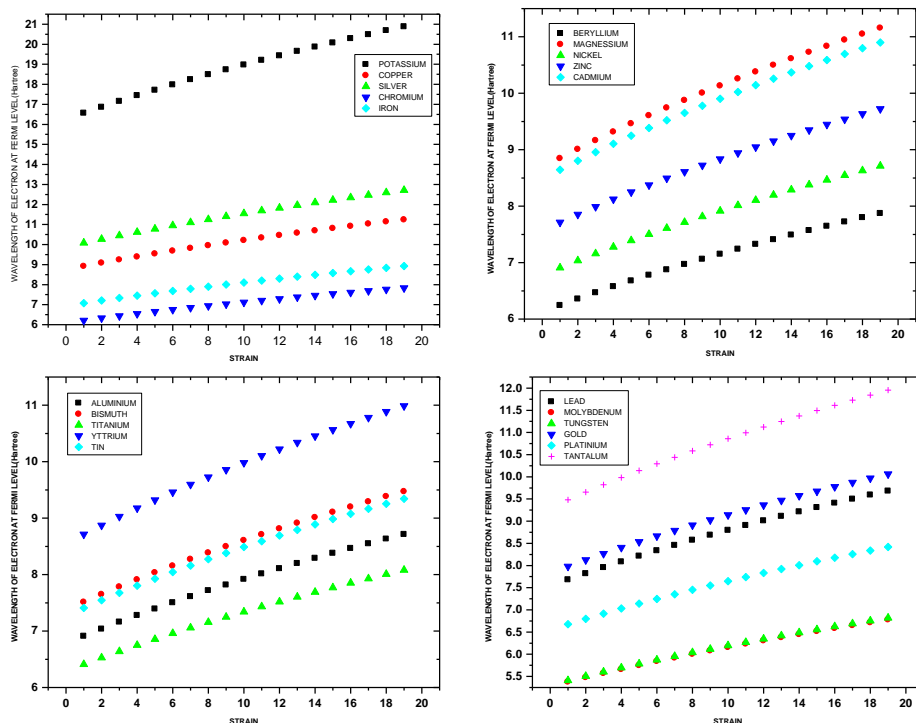


Figure 5: Wavelength of Electron at Fermi Level as a function of Strain for Metals.

Table 1: Mean Free Path of Strained (Deformed) Metals

Metals	$r_s$ (a.u)	Strain								
		0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	0.115	0.108	0.102	0.096	0.092	0.087	0.084	0.080	0.077
Cu	2.67	0.400	0.374	0.352	0.333	0.316	0.301	0.288	0.276	0.266
Ag	3.02	0.313	0.292	0.275	0.260	0.247	0.236	0.225	0.216	0.208
Be	1.87	0.516	0.482	0.454	0.429	0.408	0.389	0.372	0.357	0.343
Mg	2.65	0.257	0.240	0.226	0.214	0.203	0.194	0.185	0.178	0.171
Cr	1.86	0.522	0.488	0.459	0.434	0.412	0.393	0.376	0.360	0.347
Fe	2.12	0.401	0.375	0.353	0.334	0.317	0.302	0.289	0.277	0.267
Ni	2.07	0.421	0.394	0.370	0.350	0.333	0.317	0.303	0.291	0.280
Zn	2.31	0.338	0.316	0.297	0.281	0.267	0.255	0.244	0.234	0.225
Cd	2.59	0.269	0.251	0.237	0.224	0.213	0.203	0.194	0.186	0.179
Al	2.07	0.322	0.301	0.283	0.268	0.255	0.243	0.232	0.223	0.214
Bi	2.25	0.563	0.527	0.495	0.469	0.445	0.424	0.406	0.389	0.374
Ti	1.92	0.375	0.350	0.329	0.312	0.296	0.282	0.270	0.259	0.249
Y	2.61	0.203	0.190	0.178	0.169	0.160	0.153	0.146	0.140	0.135
Sn	2.22	0.232	0.217	0.204	0.193	0.183	0.175	0.167	0.160	0.154
Pb	2.30	0.216	0.202	0.190	0.180	0.171	0.163	0.156	0.149	0.143
Mo	1.61	0.337	0.315	0.297	0.280	0.266	0.254	0.243	0.233	0.224
W	1.62	0.376	0.351	0.330	0.312	0.297	0.283	0.271	0.260	0.250
Au	2.39	0.173	0.161	0.152	0.144	0.136	0.130	0.124	0.119	0.115
Pt	2.00	0.285	0.267	0.251	0.238	0.226	0.215	0.206	0.197	0.190
Ta	2.84	0.098	0.092	0.086	0.081	0.077	0.074	0.071	0.058	0.065

**Table 2: Wavelength of Electron at Fermi Level for Strained (Deformed) Metals**

Metals	$r_s$ (a.u)	Strain								
		0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	16.86	17.44	17.98	18.48	18.97	19.42	19.86	20.28	20.68
Cu	2.67	9.08	9.39	9.68	9.95	10.21	10.45	10.69	10.92	11.13
Ag	3.02	10.27	10.62	10.94	11.25	11.55	11.83	12.09	12.35	12.59
Be	1.87	6.36	6.57	6.78	6.97	7.15	7.32	7.49	7.65	7.80
Mg	2.65	9.01	9.32	9.60	9.88	10.13	10.38	10.61	10.83	11.04
Cr	1.86	6.32	6.54	6.74	6.93	7.11	7.28	7.45	7.60	7.76
Fe	2.12	7.21	7.45	7.68	7.90	8.11	8.30	8.49	8.67	8.84
Ni	2.07	7.04	7.28	7.50	7.71	7.92	8.11	8.29	8.46	8.63
Zn	2.31	7.85	8.12	8.37	8.61	8.83	9.05	9.25	9.44	9.63
Cd	2.59	8.80	9.10	9.39	9.65	9.90	10.14	10.37	10.59	10.80
Al	2.07	7.04	7.28	7.50	7.71	7.92	8.11	8.29	8.46	8.63
Bi	2.25	7.65	7.91	8.15	8.38	8.60	8.81	9.01	9.20	9.38
Ti	1.92	6.53	6.75	6.96	7.16	7.34	7.52	7.69	7.85	8.01
Y	2.61	8.87	9.17	9.46	9.73	9.98	10.22	10.45	10.67	10.88
Sn	2.22	7.55	7.80	8.05	8.27	8.49	8.69	8.89	9.08	9.26
Pb	2.30	7.82	8.09	8.34	8.57	8.79	9.01	9.21	9.40	9.59
Mo	1.61	5.47	5.66	5.83	6.00	6.16	6.30	6.45	6.58	6.71
W	1.62	5.51	5.69	5.87	6.04	6.19	6.34	6.49	6.62	6.75
Au	2.39	8.12	8.40	8.66	8.91	9.14	9.36	9.57	9.77	9.97
Pt	2.00	6.80	7.03	7.25	7.45	7.65	7.83	8.01	8.18	8.34
Ta	2.84	9.65	9.98	10.29	10.58	10.86	11.12	11.37	11.61	11.84

**Table 3: Mean Free Path and Wavelength of Electron at Fermi Level for Undeformed Metals**

Metals	Electron Density Parameter $r_s$ (a.u)	Experimental Fermi Energy (Hartree)	Mean Free Path (Hartree)	Wavelength of Electron at Fermi Level (Hartree)	
				Experimental Value	Computed Value
K	4.96	0.0779	42.4639	15.9062	16.2192
Cu	2.67	0.2572	36.3728	8.75384	8.73090
Ag	3.02	0.2014	37.5104	9.89246	9.87540
Be	1.87	0.5196	33.2744	6.15885	6.11490
Mg	2.65	0.2620	36.3045	8.67328	8.66550
Cr	1.86	-	33.2298	-	6.08220
Fe	2.12	0.4079	34.3347	6.95116	6.93240
Ni	2.07	-	34.1304	-	6.76890
Zn	2.31	0.4043	35.0794	6.98204	7.55370
Cd	2.59	0.2742	36.0973	8.47813	8.46930
Al	2.07	0.4274	34.1304	6.79073	6.76890
Bi	2.25	0.3638	34.8494	7.36042	7.35750
Ti	1.92	-	33.4946	-	6.27840
Y	2.61	-	36.1668	-	8.53470
Sn	2.22	0.3686	34.7326	7.31234	7.25940
Pb	2.30	0.3443	35.0414	7.56598	7.52100
Mo	1.61	-	32.0521	-	5.26470
W	1.62	-	32.1017	-	5.29740
Au	2.39	0.2025	35.3793	9.86555	7.81530
Pt	2.00	-	33.8382	-	6.54000
Ta	2.84	-	36.9385	-	9.28680



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