Theoretical Study Of The Refractive Index Of A Deformed Metal

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Abstract: In this work, a generalized model developed by Kumar and Singh (2010) for calculating the refractive index and energy band gap of different semiconducting material is extended to the study of the effect of linear deformation on the refractive index of metals by using the free electron theory to obtain the energy gap of metals and used in this work. The electron density parameters of deformed metals under the application of different strains were obtained for different metals. The poison ratio relating the transversal compression to elongation in the direction of applied deformation for different elemental metals were computed using elastic moduli for homogeneous isotropic material and used in this work. The result obtained revealed that the refractive index of metals increases as the electron density parameter increases with the metals in the high density region having low refractive index while metals in the low density region has high refractive index. This could be due to the fact that refractive index of metals depend on the electronic concentration. There is agreement between the experimental and computed value of refractive index. The experimental value used in this work is theoretically obtained from solid state physics by Charles Kittel. The refractive index of all the metals investigated in this work increases as deformation increases. This increase in refractive index of all the metals could be due to an increase in the inter-atomic spacing between the electrons in the metals which forces the refractive index of all the metals to increase as deformation increases.

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1.0 Introduction

Metals achieve structural stability by letting their valence electrons roam freely through the crystal lattice. These valence electrons are the equivalents of the molecules of an ordinary gas. It is assumed that the electrons are moving about at random and colliding frequently with the residual ions (Pillai, 2010). Refractive is like a density to an electromagnetic wave. It quantifies the speed of an electromagnetic wave through a material (Kakani and Kakani, 2004). Waves travel slower through materials with higher refractive index (Pillai, 2010). In optics, the refractive index or index of refraction n of a material is a dimensionless number that describes how light propagates through that medium. The refractive index determines how much light is bent, or refracted, when entering a material. This is the first documented use of refractive indices and is described by Snell's law of refraction. The refractive indices determine the amount of light that is reflected when reaching the interface, as well as the critical angle for total internal reflection and Brewster's angle (Rudden and Wilson, 1995). The refractive index can be seen as the factor by which the speed and the wavelength of the radiation are reduced with respect to their vacuum values. The refractive index varies with the wavelength of light. This is called dispersion and causes the splitting of white light into its constituent colors in prisms, rainbows and chromatic aberration in lenses (Vijaya and Rangerajan, 2003). The concept of refractive index is widely used within the full electromagnetic spectrum, from X-rays to radio waves. For a metallic medium the dielectric function and the index of refraction are complex valued functions. This is also the case for semiconductors and insulators in certain frequency ranges near and at absorption bands (Kachava, 1992). Many materials have a well-characterized refractive index, but these indices depend strongly upon the frequency of light. In insulators the electrons in the valence band are separated by a large gap from the conduction band, in conductors like metals the valence band overlaps the conduction band, and in semiconductors there is a small enough gap between the valence and conduction bands that thermal or other excitations can bridge the gap (Animalu, 1977). In solid-state physics, the electronic band structure of a solid describes the range of energies that an electron within the solid may have

and ranges of energy that it may not have (Kachava, 1992). Most solid substances are insulators, and in terms of the band theory of solids, there is a large forbidden gap between the energies of the valence electrons and the energy at which the electrons can move freely through the material (Pillai, 2010). Deformation can be described as change in shape or size of an object due to an applied stress (force) or strain. Metals could be deformed by a compressive, elongative and torsion/twisting force. The study of the elastic behaviour of solid is very important in the fundamental and technical researches. In technology, it tells us about the strength of the materials. In fundamental research, it is of interest because of the insight it provides into the nature of the binding forces in solids. The relevant elastic constants also relate themselves to thermal properties like Debye temperature and thermal conductivity (Kaldis, 1979). Consequently, a lot of efforts have been made to study the effect of deformation on some properties of metals theoretically and experimentally. Kumar and Singh (2010) develop a model for calculating the refractive index of different semiconductors, insulators, oxide and halides materials based on energy gap data. The calculated values of the refractive index are compared with the experimental values and the values obtained by other researchers. A fairly good agreement is obtained between them. Salah Daoud et al (2014) calculated the near neighbor distance (bond length) and the average energy gap using the pseudopotential plane wave method, in the frame work of the density functional theory (DFT) within the local density approximation (LDA) and the Hartungen- Goedecker-Hutter (HGH) scheme for pseudopotential of Boron-Bismuth compound in its structure zincblende phase and predicted the refractive index and some optoelectronic and thermal properties of boron-bismuth compound by means of some empirical formulas. The results obtained are analyzed and compared with the available theoretical data of the literature. Ahmad and Mohib-ul Hag (2014) develop a simple relation between the optical electro negativity, energy gap, refractive index and electronic polarizability for ternary chalcopyrite semiconductors. He obtained the energy gap from electro negativity while the refractive index and the electronic polarizability were obtained from the energy gap by proposing a linear relation between them. The calculated values are in agreement with the experimental values and their earlier researchers. Kiejna and Pogosov (1999) 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. Pogosov and Shtepa, (2006), calculated the surface stress and the contact potential difference of elastically deformed metals based on structureless pseudopotential model using self-consistent Kohn Sham method. The results of surface stress obtained were in agreement with experimental results, and also confirmed that the contact potential difference obtained for the deformed metallic surfaces by Kelvin method correspond to change in surface potential. Adeshakin *et. al* (2015) investigated the linear deformation and the electronic properties of metals based on the modified structureless pseudopotential model to compute and study the effects of deformation on the electron density parameter, Fermi energy, Fermi wave vector and chemical potential of different metals. The results obtained revealed that increase in deformation causes an increase in electron gas parameter, and decrease in Fermi wave vector, Fermi energy and chemical potential of metals. Adesakin, (2016) develop a model to compute the electrical conductivity of different elemental metals based on pseudopotential formalism. The results obtained revealed that there is a good agreement between the computed and experimental value of the electrical conductivity of metals. There is high concentration of electron in the high density region than the low density region. The electrical conductivity of metals decreases as deformation (strains) increases for all the metals investigated. The effect of deformation is more pronounced on the electrical conductivity of noble and transition metals than in alkaline metals. In this work, the refractive index of undeformed and deformed elemental metals of different group and period were computed and studied based on Reddy et al formalism. The results obtained for the refractive index of undeformed metal were compared with theoretical obtained experimental value to validate the model used in this work. This will provide an insight into how the refractive index of metals varies with deformation. The metals 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 Consideration

For a metal under the action of a deforming force, the average electron density in such a metal as a function of deformation is expressed as (Pogosov and Shtepa, 2006).

$$n = n_0 \left[1 - (1 - 2\upsilon) u_{xx}\right] + 0\, u_{xx}^2 \qquad (1)$$

where υ is the Poisson ratio relating compression to elongation in the direction of applied deformation, u_{xx} is the applied deformation or strain and n_0 is the average electron density in the bulk of undeformed

metal and is given as $n_0 = 3/4\pi r_s^3$ and r_s is the electron density parameter of undeformed metal. For a metal under the action of a strain or deforming force, the electron density parameter of the metal is

$$r_s[1 + (1 - 2\upsilon)U_{xx}]^{1/3} \quad (2)$$

The behaviour of electrons in the deformed metal is governed by the Schrodinger time independent equation

$$\frac{\hbar^2}{2m}\nabla^2\Psi + E\Psi = 0 \quad (3)$$

The normalized solution of equation (3) has the form (Raimes,1963)

$$\Psi = (\frac{8}{\Omega})^{1/2} \sin\left(\frac{n_x\pi}{a_x}\right)\sin\left(\frac{n_y\pi}{a_y}\right)\sin\left(\frac{n_z\pi}{a_z}\right) \quad (4)$$

The eigenvalues are given by

$$\gamma = \frac{2mE}{\hbar^2} = \pi^2\left(\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}\right) \quad (5)$$

or by

$$\gamma = k_x^2 + k_y^2 + k_z^2 = |k|^2$$

where k_x, k_y, k_z are the components of the wave vector k. In computing the quantities that requires summation over the wave vector, k the summation over k is replaced by integration according to the transformation (Raimes,1963)

$$\sum_k \rightarrow \frac{2\Omega^3}{(2\pi)^3}\int d^3k$$

The factor of two appearing in the denominator comes from the spin, According to Pauli exclusion principle, two one-electron state with opposite spins can be assigned to every k-point. In the ground state, each of the states up to the maximum, k_{max} is occupied by two electrons filling a sphere in k-space of radius k_{max} called Fermi sphere. For the system of N free electrons in the volume, Ω, the average electronic density n_{ave} in terms of k_f is

$$n_{ave} = \frac{N}{\Omega} = \frac{k_f}{3\pi^2} \quad (6)$$

The energy of the highest occupied state at absolute zero temperature is called the Fermi energy expressed as

$$E_f = \frac{\hbar^2 k_f^2}{2m} = \frac{\hbar}{2m}(3\pi n_{ave})^{2/3} \quad (7)$$

The electron gas parameter, r_{su} of the deformed metal is defined as

$$\frac{4\pi}{3}r_{su}^3 = \frac{\Omega}{N}$$

The Fermi wave vector k_f and the Fermi energy E_f of deformed metals in terms of the electron gas parameter, r_{su} is obtained as (Raimes, 1963).

$$k_f = \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_{su}} \quad (8)$$

and

$$E_f = \frac{me^4}{2\hbar^2}\left(\frac{9\pi}{4}\right)^{2/3}\left(\frac{1}{r_{su}^2}\right) \quad (9)$$

The energy band gap of deformed metals in terms of electron density parameter is obtained as

$$E_g = \left(\frac{1.9192}{r_s[1+(1-2\upsilon)U_{xx}]^{1/3}}\right)^2 \quad (10)$$

where, r_{su} is the electron density parameter for deformed metals as given by equation (2) and E_g is the energy band gap.

The expression obtained for the refractive index of deformed metals in terms of electron density parameter for a deformed metal is

$$n = \sqrt{\frac{12.417}{\left(\frac{1.9192}{r_s[1+(1-2\upsilon)U_{xx}]^{1/3}}\right)^2 - 0.365}} \quad (11)$$

where, r_s is the electron density parameter of undeformed metal, υ is the Poisson ratio relating compression to elongation in the direction of applied deformation and u_{xx} is the applied deformation or strain.

In this work, a generalized model develop by Reddy et al for calculating the refractive index of different semiconducting materials and complex binary alloy is extended to the calculation of refractive index of different elemental metals belonging to monovalent, divalent, trivalent and polyvalent group using equation (11). The energy gap used in this work is obtained using envelop function approach and how deformation affects the refractive index of metals is also studied.

3.0 Results and Discussion

Figure 1 shows the variation of refractive index with electron density parameter for some elemental metals belonging to different groups and period. Figure 1 revealed that the refractive index of metals increases as the electron density parameter increases this revealed that metals with low frequency has large refractive index while metals with large frequency has

low refractive index. Figure 1 also revealed that there is agreement between the experimental and computed value of refractive index. The experimental value used in this work is theoretically obtained from solid state physics by Charles Kittel (1976). Although, the results obtained for the refractive index of some metals gave a complex value result at some points for the electron density parameter especially during deformation. The trend exhibited by metals in figure 1 revealed that metals in the region of high density limit have low refractive index which increases towards the region of the low density limit these shows that the higher the electronic concentration of metals the lower the refractive index of the metals and the lower the electronic concentration of metals the higher the refractive of the metals. In the high density region we have the alkaline metals and the earth alkaline metals while in the low density region we have the transition and the noble metals. Figure 1 also revealed that refractive index of metals has an inverse effect on the energy gap of metals because the energy gap of metals in the high density region is high and decreases toward the low density region. Figure 2 shows the variation of refractive index with deformation for some alkaline, earth alkaline, trivalent, transition and inner transition metals. Figure 2 revealed that the refractive index of all the metals investigated increases as deformation increases. This increase in refractive index of all the metals could be due to an increase in the inter-atomic spacing between the electrons in the metals which forces the refractive index of all the metals to increase as deformation increases. The increase in the refractive index of some metals in figure 2 seems to be linear increase while some seems to exhibit a parabolic increase as these could be due to the nature of the metals. Figure 2 also revealed that metals in the high density region has low refractive index while metals in the low density region has high refractive index for all the metals subjected to different deformation. These seems to suggest that as deformation increases the lattice ion vibration about their equilibrium positions increases which results in the increase in the temperature between the interacting electron in the metals which forces the refractive index of the metals to increase as deformation increases. Figure 2 also revealed that the higher the electronic concentration in metals the lower the effect of deformation on the refractive index of the metals and the lower the electronic concentration in metals the higher the effect of deformation on the refractive index of the metals. Furthermore, the trend exhibited by metals in figure 2 revealed that as deformation increases, there is an increase in the collision between the electron due to delocalization of the electron from their equilibrium position and thereby causes an increase in the refractive index of the metals. The trend exhibited by metals in these work revealed that the refractive index of metals is greatly affected by deformation.

4.0 Conclusion

In this work, a generalized model developed by Kumar and Singh (2010) for calculating the refractive index and energy band gap of different semiconducting materials of simple and complex binary families is extended to the study of the effect of linear deformation on the refractive index of metals by using the free electron theory approach to obtain the energy gap of metals and used in this work. The result obtained shows that the refractive index of undeformed metals were in agreement with the experimental values which show the validity of the formalism used in the work. The result obtained revealed that metals in the region of high density limit have low refractive index while metals in the low density limit has high refractive index. This seems to suggest that refractive index of metals depend on the electronic concentration. The refractive index of all the metals subjected to different deformation increases as deformation increases as this could be due to an increase in the inter-atomic spacing between the electrons in the metals which forces the refractive index of all the metals to increase as deformation increases. Although. The refractive index for some metals gave a complex value results. The trend exhibited by metals in this work revealed that the refractive index of metals is highly affected by deformation.

Table 1: Refractive index 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	-	-	-	-	-	-	-	-	-
Cu	2.67	10.416	12.210	14.789	19.144	29.912	-	-	-	-
Ag	3.02	-	-	-	-	-	-	-	-	-
Be	1.87	4.503	4.756	5.009	5.264	5.521	5.782	6.049	6.323	6.606
Mg	2.65	10.101	11.741	14.021	17.635	25.159	85.695	-	-	-
Cr	1.86	4.465	4.714	4.963	5.213	5.465	5.721	5.983	6.250	6.526
Fe	2.12	5.603	5.990	6.391	6.811	7.254	7.727	8.237	8.792	9.404
Ni	2.07	5.357	5.710	6.073	6.448	6.841	7.254	7.693	8.163	8.672
Zn	2.31	6.713	7.286	7.909	8.599	9.379	10.277	11.339	12.640	14.303
Cd	2.59	9.269	10.557	12.214	14.519	18.162	25.647	75.721	-	-
Al	2.07	5.357	5.710	6.072	6.448	6.840	7.254	7.693	8.163	8.672
Bi	2.25	0.675	0.631	0.594	0.561	0.533	0.508	0.486	0.466	0.448
Ti	1.92	4.699	4.973	5.249	5.527	5.811	6.101	6.400	6.709	7.030
Y	2.61	9.529	10.919	12.749	15.388	19.855	30.886	-	-	-
Sn	2.22	6.148	6.619	7.118	7.654	8.236	8.879	9.599	10.421	11.378
Pb	2.30	6.646	7.206	7.813	8.483	9.235	10.098	11.110	12.338	13.885
Mo	1.61	3.609	3.782	3.952	4.119	4.283	4.445	4.606	4.767	4.928
W	1.62	3.640	3.816	3.988	4.157	4.324	4.489	4.653	4.817	4.981
Au	2.39	7.295	7.990	8.771	9.669	10.730	12.029	13.697	15.988	19.496
Pt	2.00	5.037	5.349	5.667	5.991	6.326	6.674	7.037	7.419	7.823
Ta	2.84	-	-	-	-	-	-	-	-	-

Table 2: Calculated Refractive Index of Undeformed Metals and their Experimental values

Metals	Electron Density Parameter r_s (a.u)	Experimental Refractive Index	Computed Refractive Index
Potassium	4.96	-	-
Copper	2.67	9.11362	9.04796
Silver	3.02	18.1296	17.8764
Beryllium	1.87	4.29128	4.24733
Magnesium	2.65	8.83563	8.82313
Chromium	1.86	-	4.21271
Iron	2.12	5.24800	5.22665
Nickel	2.07	-	5.01047
Zinc	2.31	5.29131	6.17858
Cadmium	2.59	8.23034	8.21291
Aluminium	2.07	5.03499	5.01047
Bismuth	2.25	5.85149	5.85210
Titanium	1.92	-	4.42493
Yttrium	2.61	-	8.40655
Tin	2.22	5.77589	5.69859
Lead	2.30	6.19359	6.12223
Molybdnum	1.61	-	3.42910
Tunasten	1.62	-	3.45785
Gold	2.39	17.6226	6.66135
Platinum	2.00	-	4.72647
Tantalum	2.84	-	11.6384

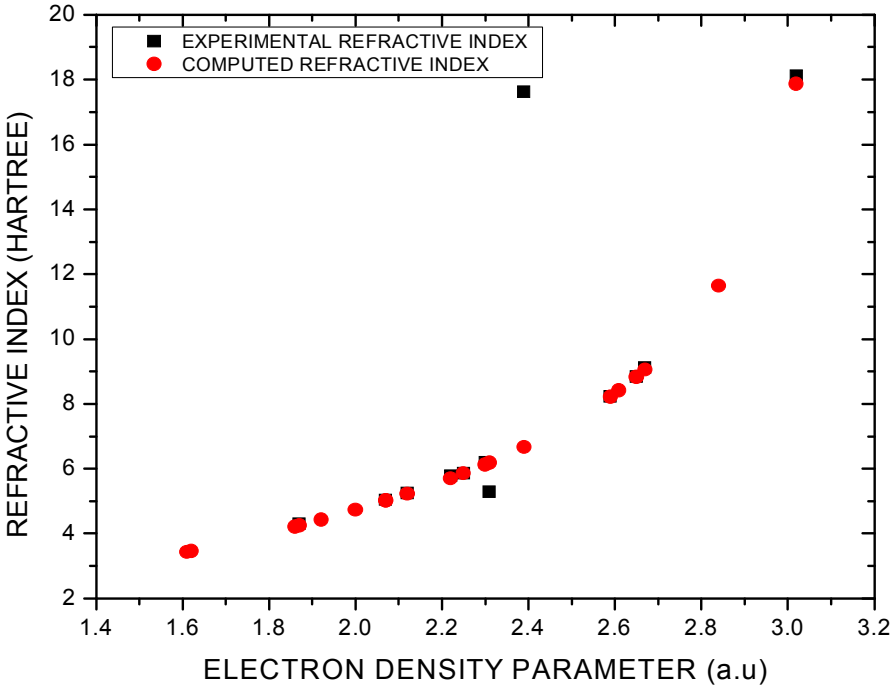

Figure 1: Variation of Refractive Index with Electron Density Parameter of Metals

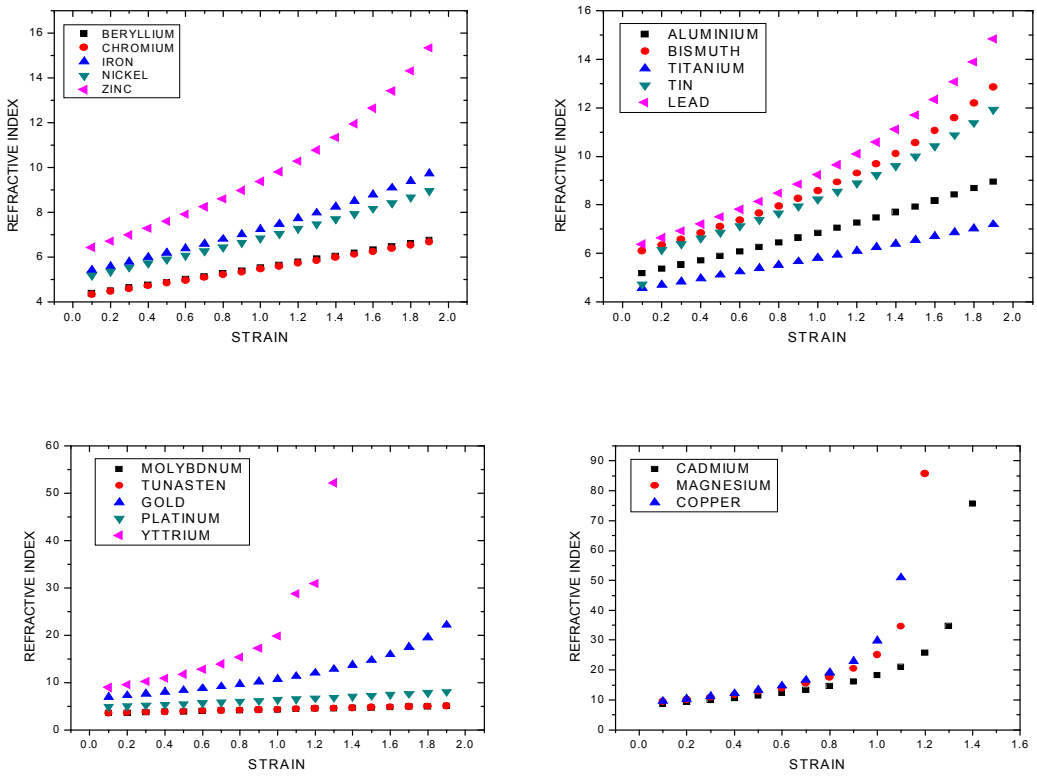

Figure 2: Variation of Refractive Index of Some Metal with Strain

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