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Coherence Length of Electron in Metals and Linear Stain based on Heisenberg Approximation using Free Electron Theory

G.E. Adesakin[1], T.H. Akande[1], O.G. Edema[2], O. O. Olusola[3], F.O. Ogunlana[3], O.A. Fasiku[1], O.D. Afe[1], Agbetuyi Oluranti Adegoke[1] and Faruq Oyediran[1]

[1]Department of Physics, Ekiti State University, Ado-Ekiti, Nigeria
[2]Department of Physical Sciences, Federal Polytechnic, Auchi, Edo State, Nigeria
[3]Department of Physics, Bamidele Olumilua University of Education, Science and Technology, Ikere Ekiti, Nigeria
G-mail of corresponding author: adesakingbenga@gmail.com

Abstract: The goal of this paper is to develop a general formulation for coherence length of electron in metal based on Heisenberg approximation using free electron theory. This study was carried out to evaluate the behaviour of coherence length of electron under strain and electron density parameter. The result obtained agree quite well with theoretically obtained experimental value. The Poisson ratio is taking into consideration during the computation. There is high concentration of electron coherence length in the region of high density limit than the low density limit. The high electronic concentration of electron coherence length in metals in the region of high density limit is due to an increase in Fermi surface of metals in the region. The electron coherence length of metal increases as the electron density parameter increases. These seems to suggest that the electron coherence length of metal relied on the cohesive and repulsive forces of electron structure of atoms and mobility of conduction electron. The electron coherence length in metals increases as the strain increases for all the metals whose electron coherence length is computed and studied due to the deviation in the electron propagation factor from their equilibrium position when strain is applied.
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Introduction

Free electron theory of metals pursues the development of ideas that lead to the understanding of various properties manifested by different materials on the basis of electronic bondings among constituent atoms Patterson and Bailey (2010). In free-electron theory, wave vector is equivalent to the momentum of electron and is quantized in the intervals of $2\pi/L$ Uichiro (2003). Due to the important role of the free electrons in binding, metals are good electrical and thermal conductor Ashcroft and Mermin (1976). Solid is a large collection of atoms that attract one another so as to confine the atoms to a definite volume of space Kachhava (1992). The term solid is mostly restricted to crystalline solids because crystalline solid are material whose atoms have a regular arrangement that exhibits translational symmetry Kittel (1976). In a regular atom arrangement, the equilibrium positions of the atoms have a regular arrangement. At any given temperature, the atoms vibrate with small amplitudes about fixed equilibrium position Animalu, (1977). Elements form solids because for some range of temperature and pressure, solid has less free energy than other states of matter. It is generally supposed that at low enough temperature and with suitable external pressure everything becomes solid Ashcroft and Mermin (1976). Metals composed of positive ion cores immersed in free conduction electrons that come from the removal of electron from an atom Pillai (2010). In metallic crystal, valence electrons are free within the constraints of the Pauli principle to wander throughout the crystal causing them to have a smoother wave function Ashcroft and Mermin (1976). In metal, Fermi surface exists and the density of states at the Fermi level is finite at absolute zero while in insulator and semiconductor, Fermi surface is absent Rogalski and Palmer (2000). The bcc, fcc and hcp structure exist most abundantly in real metals and alloys Efthimios (2003). Kinetic energy of electrons prevent metallic crystal from collapsing and compressing the solid causes the wave functions of the

electrons to "wiggle" more and hence raises their kinetic energy Kittel (1976). Coherence length characterize the spatial correlation of the paired electrons Animalu, (1977). Coherence length is a measure of the distance over which an electron propagates while maintaining its phase information Kittel (1976). Coherence length is the propagation distance of a wave from a coherent source to a point where the wave (e.g. an electron wave) maintains a specified degree of coherence Kakani and Kakani (2004). Coherence length is inversely proportional to the energy spread of electron beam Patterson and Bailey (2010). Coherence length is approximated by the ratio of speed of light in vacuum to the product of refractive index of the medium and bandwidth of the source Efthimios (2003). Coherence length is an important parameter in diffraction imaging. Coherence length in physics is the distance over which a coherent wave, like light or sound, maintains a predictable phase relationship Kachhava (1992). Superconducting coherence length is a measure of the size of a Cooper pair (distance between the two electrons). Superconducting coherence length is one of the two parameters in the Ginzburg–Landau theory of superconductivity Uichiro (2003). In superconductivity, superconducting coherence length is the characteristic exponent of the variations of the density of superconducting component Elliot (1997). Coherence is used to indicate the degree of the capability of interference of electrons emitted from an electron gun Ashcroft and Mermin (1976). A highly coherent electron source is essential for electron holography where electron waves are directly brought into interference Kakani and Kakani (2004). Coherence length is applicable in telecommunication in the transmission of messages over an electromagnetic signal, optics in the propagation of waves, such as radio waves, sound waves and compression waves and in the discussions of superconductivity, possibly because electrons can also be viewed as waves under certain conditions Madelung (1995). Some researchers have studied the coherence length of some materials using numerous computation and experimental approach. Mourachkine (2004) studied the possibility of determination of the values of coherence length and Cooper-pair size in unconventional superconductors using tunneling spectroscopy. He find that in unconventional superconductors, the inner structure of vortex core has complex structure determined by the order parameter of superconducting state and pairing wave-function of Cooper pairs. The spatial variations of order parameter and pairing wave-function occur at a distance of the order of coherence length and Cooper-pair size. He also perform tunneling spectroscopy along a line passing through a vortex core and estimated the values of coherent length and Cooper-pair size. Ohmann (2014) investigated the quantum dynamics of electrons in bulk states by scanning tunneling microscopy and spectroscopy surface using conductance maps above a threshold voltage. Theoretical calculations confirm the nature of the state elucidating the experimental findings. They observe that standing waves at step edges and defects originate from electrons in a bulk band edge at the Gamma point. From the spatially decaying waves, the wave vector and the quantum coherence parameters are determined as a function of energy. The obtained coherence length is of the order of magnitudes lower than typically observed surface potential states. The energy of the band edge is extracted from the dispersion relation and agrees with the peak measured in scanning tunneling spectra above the Fermi energy. Adesakin (2017) develop a model for computing and studying the effects of linear deformation on thermal conductivity of metals based on Debye model using kinetic theory of gas formalism. The results obtained revealed that there is a good agreement between the computed and experimental value of the thermal conductivity of metals. There is high concentration of electron in the high density region than in the lower density region which seems to suggest that thermal conductivity of metals depend on electronic concentration. The thermal conductivity of metals increases as strains increases for all the metals investigated. This could be due to an increase in the electron collision and inter-atomic distance between the interacting electrons in the metals which force the thermal conductivity of the metals to increase as strain increases. The effect of deformation is more pronounced on the thermal conductivity of alkaline metals than the noble and polyvalent metal this revealed that thermal conductivity of metals depend on electronic concentration and valence electron density. Kwon et.al (2023) investigate the coherence properties of a transmission electron microscope by analyzing Nano-diffraction speckles originating from bulk metallic glass. He obtained the spatial correlation function of the coherent diffraction patterns in the transmission geometry which reveals the highly coherent nature of the electron probe beam and its spatial dimension incident on the sample. There is a quantitative agreement between the measured speckle contrast and an analytical model which yields an estimates for the transverse and longitudinal coherence lengths of the source. He also demonstrate that the coherence length can be controlled by changing the beam convergence angle. A result that underscore the preservation of electron beam coherence throughout the electron optics as evidenced by the high-contrast speckles observed in the scattering patterns of amorphous system. Kim et.al (2009) study the spatial decay of electron coherence due to electron-electron interaction in a finite-length disorder-free quantum wire. Based on Luttinger liquid theory he demonstrated that coherence length characterizing the exponential decay

of coherence vary from region to region, and that the coherence can even be revive after the decay. The result obtained shows counter intuitive behavior which is in clear contrast to the conventional exponential decay with single coherence length due to fractionalization of an electron and the finite-size-induced recombination of the fractions.

Theoretical Consideration

The time dependence of the current I in the loop is given by

$$I(t) = I_0 \exp -\left(\frac{t}{\tau}\right) \quad (1)$$

Where I_0 is the initial value of the current and t is the elapsed time since the super-current is induced. The ratio of resistance R and self-inductance L of the superconducting loop determines the time constant τ for the current decay. Above the critical temperature T_C, metal is in the normal state and resistance R is proportional to temperature T.

Assume the usual Ohm's law (V = RI) describing the superconducting state is

$$\vec{E} = \rho \vec{J} \quad (2)$$

where $\vec{E}$ is the electric field, ρ is the resistivity and $\vec{J}$ is the electric current density, then zero resistivity implies zero electric field. So, if we take the Maxwell equation

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (3)$$

where

$$\frac{\partial \vec{B}}{\partial t} = 0 \quad (4)$$

For a superconducting state ρ = 0, $\vec{E}$ = 0. The superconducting state of metal exists only in a particular range of temperature and field strength. The condition for the superconducting state to exist in metal is that some combination of temperature and field strength is less than critical value. Superconductivity of metal disappear if the temperature of the specimen is raised above its critical temperature or if a sufficiently strong magnetic field is employed. There always exists some critical field H_c, above which superconductivity disappears. This field is temperature dependent and the empirical relation which describes well this dependence is

$$H_c(T) = H_0\left[1 - \left(\frac{T}{T_c}\right)^2\right] \quad (5)$$

where H_0 is the value of H_c at absolute zero. The specific heat C_n in a normal metal consists of electrons in the conduction band C_n^e and lattice C_n^l. Thus

$$C_n = C_n^e + C_n^i = \gamma T + \beta T^3 \quad (6)$$

The first term in equation (6) is linearly proportional to T while the second term is proportional to T^3. The specific heat of superconductor (C_{es}) at temperature well below the critical temperature T_C, the heat capacity fits an exponential form

$$C_{es}(T < T_c) = Aexp\left(-\frac{\Delta}{K_B T}\right) \quad (7)$$

Where Δ is the Fermi energy and is related to energy gap E_g as

$$E_g = 2\Delta \quad (8)$$

Such an exponential temperature dependence is the hallmark of system with gap in the spectrum of allowed energy states, separating the excited states from the ground states by energy. The relation between Fermi energy Δ and critical temperature T_C is given by Bardeen-Copper-Schrieffer (BCS) theory of superconductivity as

$$2\Delta = 3.5K_B T_c \quad (9)$$

Near the transition temperature, the half width (Δ=Eg/2) of the energy gap Eg is approximately

$$\Delta(T) = 3.2K_B T_c\left(1 - {}^{T}/_{T_c}\right)^2 \quad (10)$$

Such a temperature dependence is characteristic of a system that has an energy gap in its spectrum of allowed energy states. The Heisenberg approximation coherence length ξ is

$$\xi = \frac{\hbar v_F}{\pi \Delta} \quad (11)$$

where v_F is the Fermi velocity, $\hbar$ is normalized Planck's constant and Δ is the Fermi energy.

The motion of an electron in free space where the potential V is zero everywhere can be described by the simplest form of the Schrödinger equation

$$-\left(\frac{\hbar^2}{2m}\right)\nabla^2\varphi(x,y,z) = -\left(\frac{\hbar^2}{2m}\right)\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z) = E\varphi(x,y,z) \quad (12)$$

Where $\hbar$ the normalized Planck's constant, m is is the mass of an electron, E is energy eigenvalue and $\varphi(x,y,z)$ is total wave function expressed as $\varphi(x,y,z) = X(x)Y(y)Z(z)$. The energy of an electron in three-dimensional free space is

$$E = \left(\frac{\hbar^2}{2m}\right)\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{\hbar^2 k^2}{2m} \quad (13)$$

Equation (13) shows that the energy of an electron is proportional to the square of the wave vector k, where the wave vector k satisfies the relation

$$k^2 = k_x^2 + k_y^2 + k_z^2 \quad (14)$$

Since electron in metal must be confined in a finite space and the effect of finite size of a system on the motion of an electron is taken into account. An extension to three-dimensional space immediately leads to the wave function

$$\varphi(x,y,z) = \sqrt{\frac{1}{V}}\exp(ik.r) \quad (15)$$

and the wave vector

$$k = \left(\frac{2\pi}{L}\right)\left(n_x i + n_y j + n_z k\right) \quad (16)$$

where the wave vector k is expressed in the cartesian coordinate system with unit vectors i, j and k and integers n_x , n_y and n_z including zero. Thus, the

components k_x, k_y and k_z in wave vector k is given by $k_i = (2\pi/L)n_i$ and take discrete sets of values. The quantity V in equation (15) represents the volume of a cube with the edge length L.

Suppose the total number of free electrons per mole is equal to N_0 and the Fermi sphere with radius k_F is formed when N_0 electrons fill the reciprocal space, then the proportional relation

$$\left(\frac{2\pi}{L}\right)^3 : 2 = \left(\frac{4\pi k_F^3}{3}\right) : N_0 \qquad (17)$$

From equation (17) the Fermi wave vector k_F is obtain as

$$k_F = \left[3\pi^2 \left(\frac{N_0}{V}\right)\right]^{1/3} \qquad (18)$$

where V is the volume equal to $V=L^3$. The Fermi energy Δ with Fermi radius k_F is obtained by inserting equation (18) into equation (13)

$$\Delta = \frac{\hbar^2 k_F^2}{2m} = \left(\frac{\hbar^2}{2m}\right)\left[3\pi^2 \left(\frac{N_0}{V}\right)\right]^{1/3} \qquad (19)$$

where N_0 is obviously the total number of electrons in volume V. the electron Fermi velocity is obtained as

$$v_F = (2\Delta)^{1/2} = \left(2\left(\frac{\hbar^2}{2m}\right)\left[3\pi^2 \left(\frac{N_0}{V}\right)\right]^{1/3}\right)^{1/2} \qquad (20)$$

For metal under the action of a strain or deforming force, the electron density parameter of metal is

$$r_{su} = r_s[1 + (1 - 2\upsilon)U_{xx}]^{1/3} \qquad (21)$$

where r_s is the electron density parameter of unstrained metal, υ is the poison ratio and U_{xx} is the uniaxial strain. The coherence length ξ which estimate the average separation of electron in a cooper pair is obtained by Substituting equation (19) and (20) into equation (11) as

$$\xi = \frac{\hbar v_F}{\pi\Delta} = \frac{\hbar\left(2\left(\frac{\hbar^2}{2m}\right)\left[3\pi^2\left(\frac{N_0}{V}\right)\right]^{1/3}\right)^{1/2}}{\pi\left(\frac{\hbar^2}{2m}\right)\left[3\pi^2\left(\frac{N_0}{V}\right)\right]^{1/3}} \qquad (22)$$

where v_F is the Fermi velocity, $\hbar$ is normalized Planck's constant, Δ is the Fermi energy, m is the mass, V is the volume and N_0 is the total number of electrons. In this work, the coherence length of electron in metals were computed and studied using equation (22) base on free electron approximation theory using Heisenberg approximation.

Results and Discussion

Figure 1 shows the plot of electron density parameter dependence of electron coherence length in pure metals. Figure 1 shows that the electron coherence length of metal increases as the electron density parameter increases. These seems to suggest that the electron coherence length of metal relied on the cohesive and repulsive forces of electron structure of atoms and mobility of conduction electron. The trend display by metals in figure 1 shows that there is high concentration of electron coherence length in the region of high density limit than the low density limit this may be due to the dependence of electron coherence length of metal on the ratio of the number of valence electron in metal to the number of their atom. The result obtained in figure 1 revealed that there is a good agreement between the computed and the theoretically obtained experimental value for the coherence length of electron in metal. The trend demonstrated by metals in figure 1 indicate that the lower the value of the electron coherence length in metal the higher the electronic concentration of the metals and the higher the value of the electron coherence length in metal the lower the electronic concentration of the metals. Figure 1 also revealed that the electron separation in the cooper pair is low for metals in the region of high density limit but high for metals in the region of low density limit. Furthermore, the high electron coherence length found in metals in the region of high density limit may be due to an increase in Fermi surface of metals in the region. Figure 2 shows the plot of strain dependence of electron coherence length in pure metals. In figure 2, the electron coherence length in metals increases as the strain increases for all the metals whose electron coherence length is computed and studied. This increase in the electron coherence length as strain increases could be due to the deviation in the electron propagation factor from their equilibrium position. The increase in the electron coherence length as strain increases in figure 2 may be due to an increase in the wavelength between the interacting electrons in the metals. The increase in the coherence length of electron in metals as strain increases in figure 2 can as well be due to migration of electron from their equilibrium position as strain increases. Furthermore, the increase in the coherence length of electron in metal as the strain increases in figure 2 may be due to an increase in the inter atomic distance between the interacting electrons in metals which forced the electron in the metals to be thermally excited from their equilibrium position into higher zones leaving behind an equal number of holes and electron interlayer interaction. The trend exhibited by metals in these work revealed that the electron coherence length of metals is greatly affected by strain.

Conclusion

Coherence length of electron in metals is computed and studied based on Heisenberg approximation using the theory of free electron approximation. Result obtained revealed that the electron coherence length of metal increases as the electron density parameter increases. These suggest that the electron coherence length in metal relied on the cohesive and repulsive forces of electron structure of atoms and mobility of conduction electron. Electron coherence length in metals increases as the strain increases for all the metals whose electron coherence

length is computed and studied. This shows that as strain increases, the collision between the electrons in metal also increases which causes an increase in the electron coherence length of metals as strain increases. The increase in the coherence length of electron in metal as strain increases may be due to an increase in the inter atomic distance between the interacting electrons in metals which forced the electron in the metals to be thermally excited from their equilibrium position into higher zones leaving behind an equal number of holes and electron interlayer interaction.

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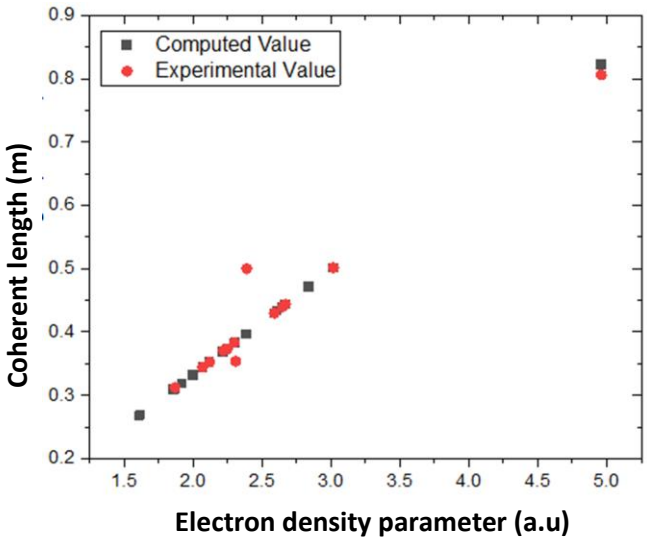

Figure 1: Plot of Electron Density Parameter Dependence of Coherence Length in Pure Metal

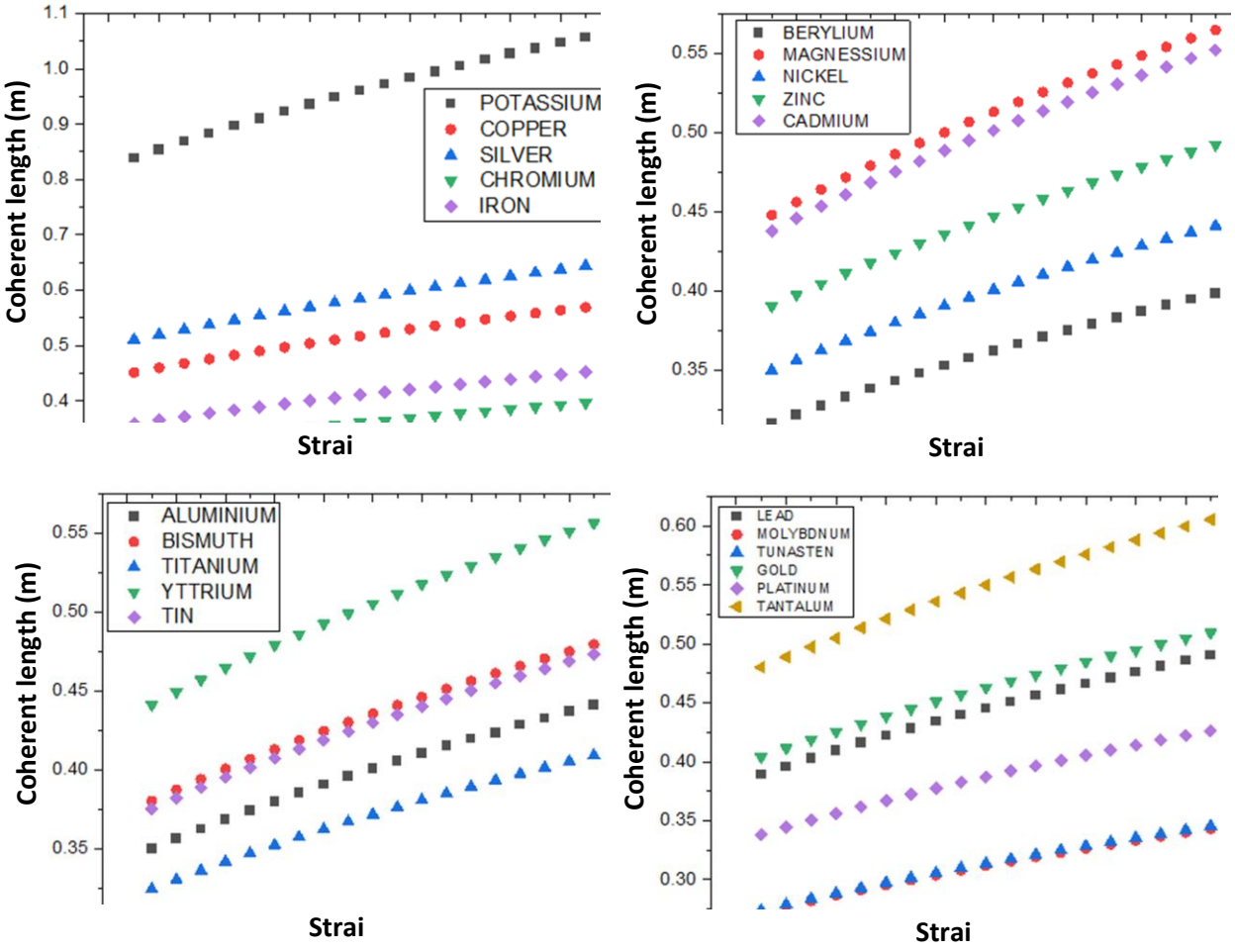

Figure 2: Plot of Strain Dependence of Coherence Length in Pure Metals

Table 1: Coherence Length of Unstrained Metals

Metals	Electron Density Parameter r_s(a.u)	Coherence Length (m)	
		Experimental Value	Computed Value
K	4.96	0.806325	0.822462
Cu	2.67	0.443755	0.442736
Ag	3.02	0.501475	0.500773
Be	1.87	0.312208	0.310081
Mg	2.65	0.439671	0.439420
Cr	1.86	-	0.308423
Fe	2.12	0.352372	0.351536
Ni	2.07	-	0.343245
Zn	2.31	0.353938	0.383042
Cd	2.59	0.429779	0.429471
Al	2.07	0.344240	0.343245
Bi	2.25	0.373119	0.373093
Ti	1.92	-	0.318372
Y	2.61	-	0.432787
Sn	2.22	0.370682	0.368118
Pb	2.30	0.383540	0.381383
Mo	1.61	-	0.266968
W	1.62	-	0.268627
Au	2.39	0.500111	0.396307
Pt	2.00	-	0.331638
Ta	2.84	-	0.470926

Table 2: Coherence Length of Strained 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	0.8538	0.8830	0.9103	0.9361	0.9605	0.9836	1.0058	1.0270	1.0473
Cu	2.67	0.4596	0.4753	0.4900	0.5039	0.5170	0.5295	0.5414	0.5528	0.5638
Ag	3.02	0.5199	0.5376	0.5543	0.5699	0.5848	0.5989	0.6124	0.6253	0.6377
Be	1.87	0.3219	0.3329	0.3432	0.3529	0.3621	0.3709	0.3792	0.3872	0.3949
Mg	2.65	0.4562	0.4717	0.4863	0.5001	0.5131	0.5255	0.5374	0.5487	0.5596
Cr	1.86	0.3202	0.3311	0.3414	0.3510	0.3602	0.3689	0.3772	0.3851	0.3927
Fe	2.12	0.3649	0.3774	0.3891	0.4001	0.4105	0.4204	0.4299	0.4389	0.4476
Ni	2.07	0.3563	0.3685	0.3799	0.3907	0.4008	0.4105	0.4198	0.4286	0.4371
Zn	2.31	0.3976	0.4112	0.4239	0.4359	0.4473	0.4581	0.4684	0.4782	0.4878
Cd	2.59	0.4458	0.4611	0.4753	0.4888	0.5015	0.5136	0.5252	0.5363	0.5469
Al	2.07	0.3563	0.3685	0.3799	0.3906	0.4008	0.4105	0.4198	0.4286	0.4371
Bi	2.25	0.3873	0.4005	0.4129	0.4246	0.4357	0.4462	0.4563	0.4659	0.4751
Ti	1.92	0.3305	0.3418	0.3524	0.3623	0.3718	0.3808	0.3893	0.3975	0.4054
Y	2.61	0.4493	0.4646	0.4790	0.4926	0.5054	0.5176	0.5293	0.5404	0.5511
Sn	2.22	0.3821	0.3952	0.4074	0.4190	0.4299	0.4403	0.4502	0.4597	0.4688
Pb	2.30	0.3959	0.4094	0.4221	0.4341	0.4454	0.4561	0.4664	0.4762	0.4856
Mo	1.61	0.2771	0.2866	0.2955	0.3038	0.3118	0.3193	0.3265	0.3334	0.3400
W	1.62	0.2789	0.2884	0.2973	0.3057	0.3137	0.3213	0.3285	0.3354	0.3421
Au	2.39	0.4114	0.4255	0.4386	0.4510	0.4628	0.4740	0.4846	0.4949	0.5046
Pt	2.00	0.3443	0.3560	0.3671	0.3774	0.3873	0.3966	0.4056	0.4141	0.4223
Ta	2.84	0.4889	0.5047	0.5212	0.5360	0.5499	0.5632	0.5759	0.5880	0.5997

cohesive and repulsive forces upon which the electron structure of atoms depends