DEVELOPMENT OF ELECTRON- POSITRON SCREENED PSEUDOPOTENTIAL

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Abstract. In the jellium model, for electron-positron annihilation to take place, the positron must overcome the screened potential of the valence electrons. In this paper, we develop electron-positron screened pseudopotential to explain positron annihilation rate in metals. The results obtained show that there is a trend in the variation of the screened pseudopotential for metals in the same group in the periodic table and also that the higher the positron annihilation rate in a metal the higher the screened pseudopotential experienced before annihilation.

1. INTRODUCTION

According to the jellium model, a solid consists of a set of interacting electrons whose total charge is balanced by a uniform rigid positive background that takes no active part in the dynamics of the system [1]. The jellium model, is a simplified type of the one electron model in which an electron is assumed to interact with the average potential generated by the other electrons and the ions. The model requires the smearing out of the background positive ions thus making the solid structureless and the positive background charge density is cancealed by an electronic contribution fixing the charge neutrality [2]. In this model, surface effect is neglected, the solid is translationally invariant and the only parameter that is retained is the electron gas parameter, r_s, which is defined as the radius of a sphere whose volume is equal to the volume per conduction electron [1-3]. It is measured in atomic units and given by the expression

$$r_s = \left(\frac{3}{4\pi v n}\right)^{\frac{1}{3}} \frac{1}{a_0} \qquad (1)$$

where v is the valency, n is the electronic concentration of the solid and a_0 is Bohr's radius. The electron gas parameter r_s, is used in the calculation of various properties of solids such as correlation energy, binding energy of the free electron gas, the kinetic energy of the valence electrons and many other properties of solids [3, 4].

Pseudopotential is a weak potential that is experienced or seen by the valence electrons [4]. It is the sum of the actual periodic potential and the repulsive potential. The pseudopotential simulates the effects of the true potential on the electrons in the conduction band [5]. The main advantage of an explicit pseudopotential model is that qualitative calculations can be performed for real crystals and results can be compared with experimental observations [4]. Various methods are used to develop or construct pseudopotential models that are used to explain various properties and phenomena in solids. Hytha and Simunek [6] presented an ab intio method for the construction of pseudopotential accommodated to a crystal environment under study. The all electron pseudopotential was based on the atomic charge density of an atom and is a functional of the crystal charge density. They used the model to calculate lattice constant and bulk moduli of silicon, diamond, face centred β-cobalt and titanium chloride. The results obtained with this model were in perfect agreement with experimental values [6].

Horsfield and Ashcroft [7] used an accurately determined energy levels obtained from low temperature galvanometric measurement of the fermi surface of aluminium to develop an empirical local pseudopotential and to test the standard scheme for calculation of band structure. They obtained an empirical pseudopotential, which gave a satisfactory result for cohesive and structural properties of aluminium metal. Pollack, Perdew and He [8] developed a density- based local pseudopotential and used it to make a comprehensive study of lattice dynamics, elastic moduli and liquid metal resistivities for 16 simple metals in the bcc and fcc crystal structures. The results obtained reveal that the phonon frequencies exhibit excellent agreement with both experimental and non-local pseudopotential theory. Also, the result shows that the buck and Voigt shear moduli are insensitive to crystal structure while the resistivity calculations confirm that electrons are scattered off the Kohn-Sham potential. Bachelet et al. [9] developed a consistent set of pseudopotentials for the whole periodic table putting relativistic effects into consideration in a way that enables the potential to be used in non-relativistic formulations. They showed a complete tabulation of the fitted potential and used the scheme to generate numerical potentials. The fitting procedure and the testing of the fit were discussed.

In this paper, we develop electron-positron screened pseudopotential and use it to explain positron annihilation rate in simple and transition metals.

2. THEORY

Consider a positively charged positron introduced into a jellium solid, specifically a metal consisting of n valence electrons each of charge ze. As the positron moves through the solid, it will

attract to itself a negative charge cloud of electrons and the electrons will correlate their motion so as to screen out the field due to the positron. In the momentum representation, the induced bare potential is [3,4]

$$\phi(b) = -\frac{4\pi ze^2}{q^2} \tag{2}$$

where z is valency and e is the charge. Since there are n electrons then,

$$\phi(b) = -\frac{4\pi zne^2}{q^2} \tag{3}$$

The screened pseudopotential [3,4] is

$$v(q) = \frac{\phi(b)}{\varepsilon(q)} \tag{4}$$

where $\varepsilon(q)$ is the Thomas- Fermi dielectric constant defined as

$$\varepsilon(q) = 1 + \frac{\lambda_s^2}{q^2} \tag{5}$$

where λ_s is the inverse of the screening length. The screening length is the distance within which the effect of the screening can be felt.

$$v(q) = \frac{4\pi zne^2}{q^2 + \lambda_s^2} \tag{6}$$

Consequently, we transform the potential into the position co-ordinate using the transform [3]

$$v(r) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} v(q) \exp(iq.r) dq \tag{7}$$

$$v(r) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{4\pi zne^2}{q^2 + \lambda_s^2} \exp(iq.r) dq \tag{8}$$

$$\therefore v(r) = \frac{-zne \exp(-\lambda_s r)}{r} \tag{9}$$

where λ_s is defined as [3] as

$$\lambda_s = \frac{2.95}{\sqrt{r_s}} \tag{10}$$

The exponential term $(\exp -\lambda_s r)$ in equation (9) is the damping factor that reduces the screening to a negligible size at distances of the order of the screening length.

In the perturbed hypernetted chain approximation, the enhancement factor is given [11] by,

$$g(r_s,0) = 1 + 1.23r_s - 0.1375r_s^2 + \frac{r_s^3}{6} \tag{11}$$

and the annihilation rate, in solid is given [12] by

$$\lambda = \frac{12}{r_s^3} \times 10^9 s \tag{12}$$

Since the positron annihilation rate is the inverse of the positron lifetime that is $\tau = \lambda^{-1}$. In this paper, the electron-positron screened pseudopotential is calculated using equation (9) above, while positron annihilation rate is calculated according to the perturbed hypernetted chain approximation (11,12). The perturbed hypernetted chain approximation is a simple and efficient method of calculating positron annihilation characteristics in metals and it provides a reasonable description of the screening of a positron for any density of the electron gas [12].

3. RESULTS AND DISCUSSION

Twenty-nine elements that are of industrial and technological applications were used to test the model. These consist of the alkaline, alkaline-earth, semi-metals and the transition metals. For the electron –positron screened pseudopotential, its variation with distance was investigated for distances between $0.1A^0$ to $6.0A^0$.For each element, results obtained are shown in Fig .1.

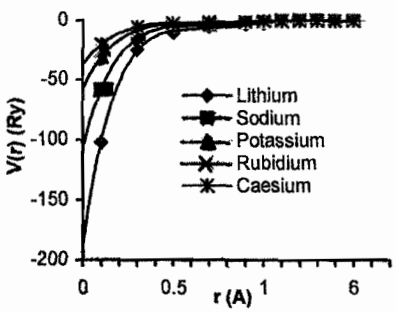

Fig. 1: Variation of screened pseudopotential with distance for group one elements

Also, in Table 1, the screened pseudopotential at $0.1A^0$ from the positron before annihilation in the solid, which is the highest value of the obtained pseudopotential for each element, is shown. The table shows that the positron annihilation rate and screened pseudopotential decrease likewise down the group for elements in the same group of the periodic table. Also, the higher the screened pseudopotential the higher is the corresponding annihilation rate. The alkaline, alkaline-earth and the group three metals of the periodic table mostly exhibit this trend. This further confirms the

experimental observation of [12] and the work of [13] about electron–positron screening affects positron annihilation characteristics in solids. This implies that the perturbed hypernetted chain approximation could be applied to positron annihilation rate in these metals.

The screened pseudopotential varies exponentially with distance in the same manner for all the elements. It has an effective value within a distance of $0.1A^{\circ}$ to $1A^{0}$ units from the positron. Subsequent data obtained for distances above $1A^{\circ}$ does not show any significant variation in the screened pseudopotential for each of the element. For distances above $1A^{0}$ units, the screened pseudopotential becomes negligible and cannot be distinguished for elements of the same group in the periodic table as shown in Figs. 1-3.

Table 1: Values of the screened pseudopotential at a distance of $0.1A^{0}$ from the positron, calculated and experimental annihilation rates for different metals. The experimental results were got from reference [13].

Metal	R_S (A.U)	$V_{0.1}A^{0}$ (R_Y)	Annihilation rate, ($x10^9$s) calculated	Annihilation rate ($x10^9$s) experimental
Li	3.25	-102.15	3.24	3.44
Na	5.95	-58.51	2.73	2.96
K	4.86	-31.40	2.38	2.52
Rb	5.20	-25.82	2.31	2.46
Cs	5.62	-20.46	2.24	2.39
Be	1.88	-499.63	7.10	7.04
Mg	2.66	-183.71	4.11	4.44
Ca	3.27	-100.04	3.22	-
Al	2.07	-376.70	5.97	6.13
Ga	2.19	-320.92	1.99	5.26
In	2.41	-243.25	1.90	5.49
Sc	-2.33	-270.26	4.97	4.35
Ti	1.92	-125.75	6.81	6.80
V	1.64	-734.34	9.13	7.69
Cr	1.86	-515.34	7.23	8.33
Mn	2.14	-342.38	5.66	-
Fe	1.84	-525.47	7.32	9.43
Co	2.08	-374.28	5.95	8.45
Ni	2.06	-381.13	6.02	9.09
Cu	2.12	-353.30	5.76	9.09
Zn	2.31	-276.17	5.03	6.76
Zr	2.11	-358.55	5.81	6.06
Nb	2.13	-348.85	5.72	8.40
Mo	1.84	-529.05	7.36	9.71
Pd	2.28	-286.37	6.66	10.42
Ag	2.40	-247.56	5.13	7.69
Cd	2.59	-197.77	4.25	5.71
Pt	2.01	-412.89	6.31	10.10
Au	2.39	-249.60	4.77	8.55
Tl	2.84	-222.92	1.87	4.76

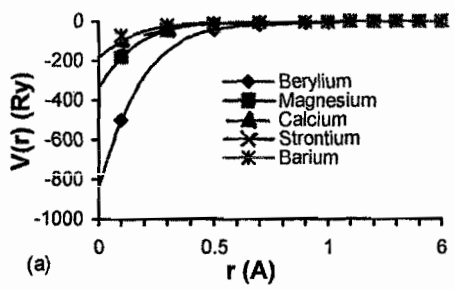

Fig.2: Variation of screened pseudopotential with distance for group two elements

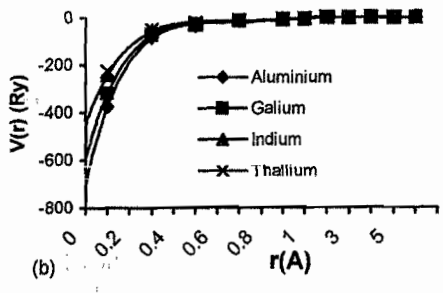

Fig.3: Variation of screened pseudopotential with distance for group three elements

4. CONCLUSION

The jellium model has been used to evaluate screened pseudopotentials and the corresponding annihilation rates of the annihilating electron–positron for groups 1, 2 and 3 elements and the transition metals. It was discovered that the higher the valence electrons of the elements, the higher the screened pseudopotential that the positron experiences in it and the higher the annihilation rate. This was in good agreement with experimental results.

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