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MODEL PSEUDOPOTENTIAL IN SIMPLE METALS

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The model potential proposed by Sharma and Srivastava has been used to study the various properties of simple metals. New core radii have also been reported corresponding to three dielectric functions. For most metals, the model potential successfully describes the atomic properties.

1. Introduction

The application of the pseudopotential technique in determining many of the physical properites of metals has proved to be very successful. In the last decade, a large number of papers have been published on this approach. An attempt towards this approach has also been made by Sharma and Srivastava [1] who have proposed a bare ion model potential for simple metals. They have obtained satisfactory results for the various properties of liquid metals [2]. In this communication several properties of solid metals have been reported. In Section 2 we shall briefly review the model potential. In Section 3 the problem of conduction electron exchange and correlation is treated. Lastly, in Section 4 calculations of properties like binding energy and compressibility, transition temperature, the Fermi surface distortion, monovacancy resistivity and third order elastic constants in simple metals have been presented. The obtained results are compared with available experimental values. In general, good agreement is achieved in theory and experiment.

2. The model pseudopotential

The Fourier transform of a bare ion pseudopotential was expressed in the form

$$W_b(q) = -\frac{4\pi ze^2}{\Omega q^2}+\frac{4\pi ze^2}{\Omega q^2}(\sin qr_c - qr_c \cos qr_c), \tag{1}$$

where z, Ω, r_c are valence, atomic volume and the radius of an ion core. In earlier studies [1], the values of core radii r_c were taken from the work of Shyu and Gaspari and Ashcroft.

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TABLE I

Core radius (r_c) for simple metals (in a.u.)

Metal	Valency	Dielectric function			
		R.P.A.	Sham	Singwi	Ref. [1]
Li	1	1.746	1.720	1.694	1.678
Na	1	1.551	1.546	1.536	1.758
K	1	1.871	1.864	1.854	2.133
Rb	1	2.080	—	—	2.256
Al	3	1.060	1.053	—	1.131
Pb	4	1.065	1.075	—	1.075

In this paper, the parameter r_c has been determined by fitting $V(q) = W_b(q)/\varepsilon(q)$ to the experimentally determined point [3] at q equal to the (110) and (111) reciprocal lattice vector for b.c.c. and f.c.c. metals respectively. The core radii r_c corresponding to three dielectric functions have been reported in Table I. The screened form factors in the present study and in Sharma and Srivastava [1] possess a similar trend at low q values but our form factors decrease rapidly at large q values.

3. *The dielectric screening*

The problem of exact analysis for the response of an electron gas at metallic densities is difficult. In recent years, a great deal of attention has been given to the problem of a homogeneous gas of interaction electrons. The most commonly used dielectric is the Hartree dielectric function which later has been modified by various authors who have suggested different expressions for exchange and correlation. In the present work we have used the modified Hartree dielectric function which is given by

$$\varepsilon(q) = 1 + \frac{4\pi z e^2}{\Omega q^2}(1-f(q))\frac{3}{2E_F}\left[\frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q}\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right]. \tag{2}$$

The function $f(q)$ corrects for exchange and correlation effects. In the present calculations we have used three different forms of $f(q)$:

(1) the Random Phase Approximation proposed by Linhard [4]

$$f(q) = 0;$$

(2) an expression introduced by Sham [5]

$$f(q) = q^2/2(q^2 + k_F^2 + k_S^2)$$

(3) the expression given by Singwi et al. [6] who have included the effect of the local field in a self consistent way

$$f_{\mathrm{SSTL}}(q) = A[1 - \exp\{-Bq^2/k_F^2\}].$$

4. *Results and discussions*

4.1. Binding energy and compressibility

Considering the free electron approximation and the perturbation theory, the binding energy and compressibility were calculated using the expression of Saxena et al. [7]. The overlap repulsion between ion cores was neglected

$$E_b = \frac{0.737}{r_S^2} - \frac{2}{3}\left(\frac{0.916+1.792z^{2/3}}{r_S}\right) - 0.105 + 0.031 \ln r_S$$
$$+ \frac{3}{16\pi^2(12\pi^2)^{1/3}} \frac{1}{r_S^4} \sum_{q\neq 0} \frac{|W_b(q)|^2}{2T} \ln\left|\frac{1+T}{1-T}\right|, \tag{3}$$

$$\frac{k_0}{k} = \frac{1}{22.1}\Bigg[0.093 r_S^2 + 2(0.916+1.792z^{2/3}) r_S - 4.42$$
$$+ \frac{9}{32\pi^2(12\pi^2)^{1/3}} \frac{1}{r_S^2} \sum_{q\neq 0} \frac{2|W_b(q)|^2}{1-T^2}\left(1 - \frac{5(1-T^2)}{2T} \ln\left|\frac{1+T}{1-T}\right|\right)\Bigg] \tag{4}$$

and $T = q/2k_F$

TABLE II

Theoretical and experimental values of binding energy and compressibility

Metal	Binding energy Ry/electron ($-E_b$)		Compressibility (k/k_0)	
	Theoretical	Experimental	Theoretical	Experimental
Li	0.550	0.551	1.65	2.0
Na	0.470	0.460	1.30	1.5
K	0.396	0.390	1.08	1.0
Rb	0.371	0.366	0.900	0.82

The calculated values are listed in Table II. The results seem to be in good agreement with experiment. It is seen that a small change in the core radius due to the dielectric constant does not make an appreciable change in the value of the binding energy and compressibility.

4.2. Transition temperature

McMillion [8] has derived an approximate solution of the Nambu–Gorkov [9, 10] equations and obtained a simple formula for the transition temperature T_c as a function of the electron-phonon mass enhancement λ and the Coulomb coupling μ^* as

$$T_c = \frac{\theta_D}{1.45} \exp\left[-\left(\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)\right], \tag{5}$$

$$\mu^* = \frac{\mu}{1+\mu \ln (E_F/k\theta_D)}, \tag{6}$$

$$\mu = \frac{1}{\pi k_F} \int_0^{2k_F} \frac{dq}{q\varepsilon(q)}, \tag{7}$$

where θ_D is the Debye temperature, k_F the Fermi wave vector, E_F the Fermi energy and $\varepsilon(q)$ the dielectric function for momentum transfer q.

The parameter λ which provides a direct measure to the electron-phonon coupling strength has been calculated by various workers for simple metals using a variety of approaches. Seven such calculations have been summarized by Allen and Cohen [11] which showed that, at least for simple metals, the most naive calculations give the same result as the most complex. The expression for λ is given by Rajput and Gupta [12] as

$$\lambda = \frac{m\Omega_0}{4\pi^2 k_F M k^2 \theta_D^2} \int_0^{2k_F} \frac{q^3}{\varepsilon^2(q)} W_b^2(q)dq, \tag{8}$$

where Ω_0 represents the atomic volume, M the atomic mass, $W_b(q)$ the bare pseudopotential. The calculated values of the mass enhancement λ, the Coulomb pseudopotential μ^* and the superconduction transition temperature T_c are given in Table III and compared with experimental results. The agreement between the theoretical and experimental values of the T_c is comparable for aluminium and lead. No experimental results are available for T_c of alkali metals, however our present calculations are in agreement with other theoretical values [11, 13] and predict that alkali metals behave as normal metals. To conclude, we can therefore say that the present model potential is successful in interpreting the superconduction state parameters.

TABLE III

Calculated values of the superconducting state parameters

Metal	θ_D (K)	μ^* R.P.A.	μ^* Sham	λ R.P.A.	λ Sham	T_c R.P.A.	T_c Sham	T_c Experimental
Li	335	0.1200	0.1245	0.2211	0.2530	7.1×10^{-5}	0.0014	<0.08
Na	156	0.1180	0.1222	0.2240	0.2821	7.2×10^{-5}	0.0071	
K	91	0.1198	0.1237	0.2080	0.2633	1.9×10^{-6}	0.0001	
Al	423	0.1023	0.1058	0.3841	0.4550	1.1	2.0	1.196
Pb	102	0.0927	0.0955	0.8686	1.038	5.0	6.5	7.23

4.3. The Fermi surface distortion

Experimental [14, 16] and theoretical [17–25] studies have yielded information about the anisotropies of Fermi surfaces of simple metals i.e. the Fermi surface should be slightly distorted from a free electron sphere and the distortion should increase in the sequence

Na, K, Rb, Cs. The electronic band structure is determined by the secular equation

$$\det \left| \left[\frac{\hbar^2}{2m}(k-q)^2 - E_k \right] \delta_{qq'} + F(q-q')V(|q-q'|) \right| = 0, \tag{9}$$

where $F(q-q')$ is the structure factor. The distortion of the Fermi surface from a free electron sphere may be written as

$$k_F = k_F^0[1+\Delta(\theta)]. \tag{10}$$

Here θ is the angle between k_F and q and k_F^0 is the free electronic Fermi wave number. Thus $\Delta(\theta)$ is the dilation to the free electron Fermi radius k_F^0. From second order perturbation theory we can write

$$E_F = \frac{\hbar^2}{2m} k_F^{02} - \sum_{q\ \mathrm{pairs}} C(q)\,|V(q)|^2. \tag{11}$$

To evaluate $C(q)$, we make use of the condition that the distortion should not alter the volume enclosed by the Fermi surface. Elementary integration yields

$$C(q) = \frac{m}{2\hbar^2 k_F^0 q} \ln \left| \frac{2k_F^0+q}{2k_F^0-q} \right|. \tag{12}$$

The quantity $\Delta(\theta)$ is small and hence higher powers of $\Delta(\theta)$ are neglected. We find

$$\frac{\Delta k_F}{k_F^0} = \sum_{q\ \mathrm{pairs}} \frac{|V(q)|^2}{E_F^0} \left(\frac{1}{(\hbar^2/2m)q^2 - 4E_F^0 \cos\theta_{kq}} - C(q) \right), \tag{13}$$

which indicates that the deviation from sphericity are simply additive and any number of the Bragg plane pairs can be considered. In the present calculation the summation has been done up to the 8th neighbour for reciprocal lattice vectors.

The radial distortion of the Fermi surface of Li, Na and K along the (100), (110) and (111) directions are calculated using equations (11) and (13). The values of x, y and δ are also calculated from the distortions along the (100), (110) and (111) dorections. The calculated values are presented in Table IV and compared with the experimental values. The agreement between the calculated and experimental values is reasonable. The radial distortion of the Fermi surface is found to be too small for alkali metals which shows that the Fermi surface of alkali metals is nearly spherical. In the present calculation the value of effective mass is considered to be a unity. It can be clearly seen in Table IV that the values of Y for Li, Na and K obtained from the present calculation are better than the recent calculation of So et al. who have included the effect of effective mass in terms of bare mass and the electron-phonon coupling parameter. Our calculated values of x for Na and K are to be found poorer than So et al.'s results. It is important to note that the calculated value of the radial distortion δ for Li is extremely good and very close to the

TABLE IV

Values of the radial distortion of fermi surfaces in $\Delta k_F/k_F^0 \times 10^2$; $X = (k_{100}-k_{111})\, k_F^{0^{-1}} \times 10^2$; $Y = (k_{110}-k_{111})\, k_F^{0^{-1}} \times 10^2$ and $\delta = (k_{110}-k_{100})\, k_F^{0^{-1}} \times 10^2$

Metal	References	Modified dielectric function	(100)	(110)	(111)	X	Y	δ
Li	our work	Sham	−1.48	+1.82	−0.37	−1.11	+2.19	3.30
	our work	Singwi et al.	−1.60	+1.97	−0.40	−1.20	+2.37	3.57
	Ham		—	—	—	−1.00	+4.00	5.00
	Dangen and Perrot		−2.51	+2.32	−1.37	−1.14	+3.69	4.83
	Inoue et al.		−2.18	+2.90	−0.97	−1.21	+3.87	5.08
	Matsuura (OMP)		—	—	—	—	—	7.61
	So et al.		—	—	—	−1.59	+4.16	5.75
	Experiment (Randles and Springford)		—	—	—	—	—	2.6±0.9
Na	our work	R.P.A.	−0.035	+0.088	−0.027	−0.008	+0.115	0.123
	our work	Sham	−0.032	+0.084	−0.026	−0.006	+0.110	0.116
	our work	Singwi et al.	−0.029	+0.080	−0.020	−0.009	+0.100	0.109
	Schneider and Stoll		−0.06	+0.084	−0.024	−0.036	+0.108	0.144
	Ho		−0.008	+0.017	−0.010	+0.002	+0.027	0.025
	So et al.		—	—	—	−0.089	+0.048	0.137
	Matsuura (OMP)		—	—	—	−0.11	+0.18	0.290
	Experiment		−0.078	+0.093	−0.015	−0.063	+0.108	0.171
K	our work	R.P.A.	−0.144	+0.253	−0.10	−0.044	0.353	0.397
	our work	Sham	−0.133	+0.236	−0.098	−0.035	0.334	0.369
	our work	Singwi et al.	−0.121	+0.212	−0.087	−0.034	0.299	0.333
	Schneider and Stoll		−0.203	+0.252	−0.053	−0.150	0.305	0.455
	Matsuura (OMP)		−0.204	+0.009	+0.005	−0.029	+0.004	0.033
	Ham		—	—	—	0.0	+1.30	1.30
	So et al.		—	—	—	0.258	+0.093	−0.165
	Experiment		+0.147	+0.108	−0.110	0.257	+0.218	−0.039

recent experimental value of Randles and Springford [16]. It is surpising that the distortion of K along the (100) direction in experiment is found to be positive while it is negative in the case of Li, Na and Rb.

4.4. Monovacancy resistivity

The monovacancy resistivity within the framework of the pseudopotential formalism can be calculated as has been attempted by various workers [26, 27]. The expression is

$$\varrho = \frac{3\pi\Omega}{V_F^2 \hbar e^2} \langle |V(q)|^2 \rangle,$$

where

$$\langle |V(q)|^2 \rangle = \frac{1}{4k_F^4} \int_0^{2k_F} |V(q)|^2 q^3 dq, \tag{14}$$

where V_F is the Fermi velocity and $V(q)$ is the pseudopotential matrix element screened by the dielectric constant.

Monovancancy resistivity of simple metals are presented for three dielectric constants in Table V. No reasonable comparison between theory and experiment is possible here due to the lack of experimental results. For comparison, the theoretical results obtained by Shyu et al. [26] using Singwi et al.'s [6] screening are also listed. Harrison [28] has also calculated ϱ in Al to be 0.8 μΩ cm/at % using Hartree dielectric screening. Some discrepancies may arise here from neglecting lattice distortion and assuming that the vacancy concentration is small, so that one has essentially a collection of singly isolated vacancies. It can be seen that the calculated values of monovacancy resistivity are better for Singwi et al.'s dielectric constant. Similar trend has been obtained by Shyu et al.

TABLE V

Resistivity of vacancies in simple metals in μ Ω cm/at %

Dielectric function	Li	Na	K	Al	Pb
R.P.A.	0.43	0.80	1.25	0.48	0.80
Sham	0.49	1.01	1.58	0.57	0.98
Singwi et al.	0.52	1.20	1.86	0.68	1.1
Ref. [21]	0.76	1.13	1.53	0.67	—

4.5. Third order elastic constants of sodium and potassium

While considerable work has been done with sufficient success in the study of second order elastic constants of alkali metals [29–31] by both theoretical and experimental workers, much less attention has been paid to the study of third order elastic constants (TOE). There are two methods for calculating the elastic constants, the long wave method and the homogeneous deformation method. The method of homogeneous deformation was extended to third order elastic constants of alkali metals by Suzuki et al. [32] using the model potential of Ashcroft, Suzuki et al. did not use any correction for exchange and correlation in the dielectric screening. The exchange and correlation will influence up to three Fuchs' third order elastic constants which measure the volume derivatives of the second order elastic constants. Therefore all the Brugger elastic constants will be effected even though only three Fuchs' elastic constants would be changed.

Srinivasan and Girirajan [33] have used the longwave method to determine the second and third order elastic constants of alkali metals. They have used the Heine-Abarenkov and Wallace potentials with different exchange and correlation corrections. In this paper, a calculation of the third order elastic constants of Na and K, based on the method of homogeneous deformation is presented. In view of the significant role played by exchange and correlation in elastic constants, we have included the dielectric function in the present calculation. The procedure used here is closely parallel to that of Suzuki et al. except for the use of slightly different deformation parameters. The deformation tensors used here are

$$\alpha_{ij}(\chi) = \begin{pmatrix} \chi^{1/3} & 0 & 0 \\ 0 & \chi^{1/3} & 0 \\ 0 & 0 & \chi^{-2/3} \end{pmatrix}; \quad \alpha_{ij}(\lambda) = \tfrac{1}{3}\lambda^{1/3} \begin{pmatrix} \lambda^{-1}+2 & \lambda^{-1}-1 & \lambda^{-1}-1 \\ \lambda^{-1}-1 & \lambda^{-1}+2 & \lambda^{-1}-1 \\ \lambda^{-1}-1 & \lambda^{-1}-1 & \lambda^{-1}+2 \end{pmatrix}$$

and

$$\alpha_{ij}(k) = k^{1/3} \begin{pmatrix} \frac{1}{2}(k^{-1}+1) & \frac{1}{2}(k^{-1}-1) & 0 \\ \frac{1}{2}(k^{-1}-1) & \frac{1}{2}(k^{-1}+1) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{15}$$

where deformations χ, λ, k contract the lattice along the (001), (111) and (110) directions respectively and expand it in the plane perpendicular to these directions so as to maintain constant volume. In addition, we require a deformation defining a simple volume change as $\alpha_{ij} = v^{1/3}\delta_{ij}$ where v is the reduced volume $v = V/V_0$. Thus the elastic constants are determined from the derivatives of total energy with respect to the above mentioned deformation parameters and the Fuchs' TOE ($C_{\chi\chi\chi}$, $C_{\lambda\lambda\lambda}$ etc.) thus obtained are converted to Brugger's TOE ($C_{111}, C_{112}, \ldots$ etc.) using the relations given by Thomas [34], we have used the Hartree screening function corrected for the exchange and correlation on the lines of Sham [5]. The parameter r_c in the model potential has been chosen to fit the second order elastic constants to their experimental values. The obtained values are $r_c = 1.597$ for sodium and $r_c = 1.748$ for potassium. The calculations are extended to the first five sets of reciprocal lattice vector. The value of α in a free electron energy is determined through the condition $dE/dr_S = 0$ to assure the crystal equilibrium at the observed lattice spacing. The band structure energy is found to make a small contribution to the second order elastic constants but an indispensable contribution to the third order elastic constants. Besides the dielectric function and exchange and correlation, the band structure energy

TABLE VI

Third order elastic constants (10^{11} dyn/cm^2) of Na and K as a function of core radius (a.u.)

Core radii	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
			Sodium			
1.50	−6.73	−1.59	−2.21	−1.80	−1.37	−1.61
1.55	−6.83	−1.58	−2.18	−1.77	−1.39	−1.63
1.60	−7.01	−1.65	−2.27	−1.81	−1.38	−1.70
1.65	−7.11	−1.71	−2.31	−1.95	−1.38	−1.81
1.70	−7.40	−1.96	−2.36	−2.04	−1.37	−1.94
			Potassium			
1.60	−3.62	−0.45	−1.15	−0.41	−1.03	−1.07
1.65	−3.70	−0.49	−1.08	−0.43	−1.02	−1.08
1.70	−3.88	−0.54	−1.25	−0.45	−0.99	−1.12
1.75	−4.09	−0.58	−1.63	−0.48	−0.98	−1.20
1.80	−4.44	−0.62	−1.96	−0.51	−0.98	−1.28
1.85	−4.87	−0.70	−2.32	−0.56	−0.98	−1.38

mainly depends upon the model potential used. This model potential contains the core radius as the only adjustable parameter. So it may not be out of place to find the effect of the core radius on the individual third order elastic constants. The third order elastic constants as the function of core radius are listed for sodium and potassium in Table VI. It may be noted that the predicted sets of third order constants of Na and K have the common features that the magnitude of C_{111} is appreciably larger than that of other constants. We also see that the maximum variation of elastic constants with core radius is observed for C_{111} and minimum for C_{166}. The calculated values, except C_{144} of K, are found to be in reasonable agreement with theoretical calculations of Suzuki et al. and Srinivasan and Girirajan. However, no exact conclusion can be drawn as there are no experimental data available for Brugger's third order elastic constants of alkali metals.

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