

Pseudopotential calculations for simple metals

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(Received 14 November 1977)

The model pseudopotential proposed by the author is used to calculate the binding energy, compressibility and monovacancy resistivity of simple metals. The screened form factors of the potential are presented for Na, K, Rb, Cs and are compared with those obtained by Shyu *et al*.

1. INTRODUCTION

Pseudopotential theory has been remarkably successful in the calculation of atomic properties of simple metals. The general procedure (Harrison 1963) of determining these properties is to start with the total energy which is the sum of three contributions, viz. the modified free electron energy, the electrostatic energy and the band structure energy. The band structure energy represents the deviation of the energy of the conduction electrons from that of a free electron gas. It is calculated from the second-order perturbation energy of a conduction electron in an expansion of the pseudopotential and can be written as

$$U_{bs} = \sum'_{\mathbf{q} \neq \mathbf{G}} F(\mathbf{q}) \quad \dots (1)$$

where $F(\mathbf{q})$ is called the energy wave number characteristic, \mathbf{G} is a reciprocal lattice vector and the prime on the sum indicates that the term with $\mathbf{G} = 0$ is excluded.

During the last few years, considerable information has been obtained for the electron ion potential by empirical fitting of the Fermi surface data and many model pseudopotentials have been suggested by various workers. However, it is well known that one can always find a suitable model potential to interpret specific properties because each property is related to the Fourier transform of the potential in a certain range of momentum transfer.

2 THE MODEL PSEUDOPOTENTIAL

The potential has generally been expressed in the model form containing few adjustable parameters. In an earlier paper Khanna (1977) a simple expression

for bare-ion pseudopotential is proposed to describe the electron-ion interaction in simple metals of the form

$$W_b(q) = \frac{2\pi Z e^2}{\Omega q^2} \left(-\cos(qr_c) - \frac{\sin(qr_c)}{qr_c} \right) e^{-0.026 q^4} \quad \dots (2)$$

where Z , Ω , r_c are valence, atomic volume and the radius of ion core. The first term arises from the long range Coulomb field of the net ion charge Ze . The second term represents the contribution from the ion core region. The limiting value of $W_b(q)$ as q goes to zero is $-4\pi Z e^2/\Omega q^2$ which satisfies the correct limit required by charge neutrality. The parameter r_c has been determined by fitting $V(q) = W_b(q)/E(q)$ to the experimentally determined point at q equal to the (110) and (111) reciprocal lattice vectors for bcc and fcc metals respectively (Setz *et al* 1970). The term $\exp(-0.026q^4)$ has been included here to improve the convergence of the potential for higher values of q . The coefficient in the exponent was arbitrarily chosen so that the form factor decreases rapidly after $q = 5 K_F$. To take into account the effect of screening, the Hartree dielectric function has been used. The exchange and correlation effects are considered on the lines of Sham (1965). For $E(q)$, the following formula was used

$$E(q) = 1 + \frac{4\pi Z e^2}{\Omega q^2} [1 - q^2/2(q^2 + K_F^2 + K_S^2)] S(q)$$

$$S(q) = \frac{3}{2 E_F} \left[-5 + \frac{4 K_F^2 - q^2}{8 K_F Q} \ln \left| \frac{2 K_F + q}{2 K_F - q} \right| \right] \quad \dots (3)$$

where E_F and K_F are the energy and wave number of an electron at the Fermi surface respectively, K_S is the Thomas-Fermi screening vector

3 BINDING ENERGY AND COMPRESSIBILITY

Considering the free electron approximation and the perturbation theory, the binding energy and compressibility were calculated using the expression given by Saxena *et al* (1969). The overlap repulsion between ion cores were neglected

$$E_b = \frac{0.737}{r_S^2} - \frac{2}{3} \left(\frac{0.916 + 1.792 Z^{2/3}}{r_S} \right) - 0.105 + 0.031 \ln r_S$$

$$+ \frac{3}{16\pi^2 (12\pi^2)^{1/3}} \frac{1}{r_S^3} \sum_{q \neq 0} \frac{|W_b(q)|^2}{2T^3} \ln \left| \frac{1+T}{1-T} \right| \quad \dots (4)$$

$$\frac{K_0}{K} = \frac{1}{22.1} \left[0.089 r_S^2 + 2(0.916 + 1.792 Z^{2/3}) r_S - 4.4^2 \right]$$

$$+ \frac{9}{32\pi^2 (12\pi^2)^{1/3}} \frac{1}{r_S^2} \sum_{q \neq 0} \frac{2 |W_b(q)|^2}{1-T^2} \left\{ 1 - \frac{5(1-T^2)}{2T} \ln \left| \frac{1+T}{1-T} \right| \right\} \quad \dots (5)$$

where, $T = q/2K_F$

4. RESISTIVITY OF VACANCIES OF SIMPLE METALS

It is simple to calculate the monovacancy resistivity within the frame work of pseudopotential formalism as has been attempted by various workers Shyu *et al* (1971), Behari (1973). The expression is

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

where,

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

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

5 RESULTS AND DISCUSSIONS

Using this model potential, the form factors of effective electron-ion potential are determined for alkali metals and shown in Fig. 1. This form of pseudopotential

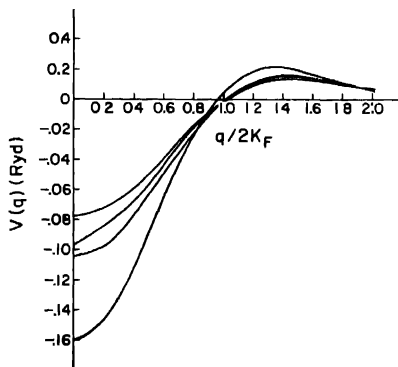


Fig. 1 The screened form factors of alkali metals.

is superior to various existing pseudopotentials in the sense that the oscillations in form factors decreases considerably for large momentum transfer. The form factors of Na and K of Shyu *et al* (1971) are shown in Fig 2. It can be seen that in the wave vector region between $q = 0$ and $2K_F$ their plots are in broad agreement with those of the author. The contribution from this region plays a dominant part in the calculation of most of the dynamical properties.

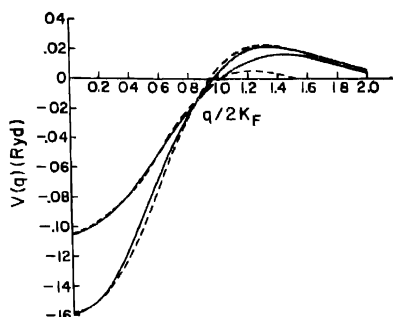


Fig 2 Comparison of our form factors with Shyu *et al* Khanna's full lines, Shyu *et al* broken lines.

Table 1 CORE RADII IN ÅU

Metal	Core radius r_c
Na	2.15
K	2.53
Rb	2.71
Cs	2.90
Al	1.50
Pb	1.30

Table 2 Theoretical and experimental values of binding energy and compressibility

Metal	Binding energy in Ry/electron ($-E_b$)		Compressibility K/K_0	
	Theoretical values	Experimental values	Theoretical values	Experimental values
Na	474	460	1.32	1.50
K	396	390	0.92	1.00
Rb	370	366	0.84	0.82
Cs	349	345	0.76	0.78

The binding energy and compressibility were calculated from eqs (4) and (5) respectively and are listed in table 2 along with the experimental values. The calculated values are in good agreement with the experimental values.

Monovacancy resistivity of simple metals are presented in table 3. No reasonable comparison between theory and experiment is possible here due to the lack of experimental results. For comparison, theoretical results obtained by Shyu *et al* (1971) using Hartree screening are also listed. Harrison (1966) has also calculated ρ_v in Al to $0.8 \mu\Omega$ cm/at% using Hartree screening. Some discrepancies may arise here from the neglect of lattice distortion and assumes the vacancy concentration to be small so that one has essentially a collection of simply isolated vacancies.

Table 3 Resistivity of vacancies in simple metals in $\mu\Omega$ cm/at%

Metal	Present calculation	Results of Shyu <i>et al</i> calculation
Na	0.67	0.77
K	0.98	1.00
Rb	1.06	
Cs	1.21	
Al	0.44	0.52
Pb	0.86	1.64 ^a , 0.56

^a See Behari (1973).

6 CONCLUSIONS

It may be concluded that this model potential is able to interpret the dynamical properties in a satisfactory manner. By introducing a damping factor we have been able to bring its form factors more in accordance with the physically acceptable situation.

ACKNOWLEDGMENTS

The author is thankful to Dr. P. K. Sharma, Allahabad University for valuable suggestions.

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