YU ISSSN 0015—3206
FZKAAA 14 (4) 241 (1982)

THE EFFECT OF INTRODUCING A LARGE-MOMENTUM-TRANSFER CUTOFF IN THE PSEUDOPOTENTIAL CALCULATIONS OF THE ENERGY BAND STRUCTURE AND RESISTIVITY OF LIQUID Al AND Pb

N. VUKOTIĆ

Teacher's Training College, University »Veljko Vlahović«, 81400 Nikšić, Yugoslavia

Received 1 June 1982

Revised manuscript received 6 July 1982

UDC 538.93

Original scientific paper

Energy bands and liquid metal resistivities of Al and Pb are determined using a modified form of a general model pseudopotential[1]. The results obtained are in a very good agreement with the available experimental data for these metals.

1. Introduction

There are some situations in which it is important to have an analytical form of the pseudopotential form factor $v(q)$. Such examples are: the calculations of liquid metal resistivities, problems in which the translational symmetry has been broken by a perturbation, precise calculations of energy band structure in the framework of local approximation etc.

General model pseudopotential[1] method has been successfully applied in the investigations of some features of metals[2,3,4], alloys and some biological systems[5]. However, the investigation of aluminium energy bands using general model pseudopotential has not produced satisfactory results.

One of the shortcomings of such a pseudopotential is a weak convergence in the range of high q-values, having as a consequence of weakly damped oscillating tail. One type of a modification of the general model pseudopotential[6] has given satisfactory results in energy band calculations of Al. Following this idea, a change of the form factor of general model pseudopotential[1] is proposed in the present work by introducing a single additional parameter β_3, in the matrix element:

$$\langle \vec{k} + \vec{q}\, |v|\, \vec{k} \rangle = \beta_1 \beta_2 \frac{\sin 2\pi \beta_2 q/2K_F}{2\pi \beta_2 q/2K_F} \exp(-\beta_3 q/2K_F). \tag{1}$$

The values of the parameters β_2 and β_3 are determined from the experimental form factors[7,9] as follows (1 Ry = 13.6 eV):

Al: $v(111) = 0.0179$ (Ry) $\quad v(200) = 0.0562$ (Ry)

Pb: $v(111) = -0.084$ (Ry) $\quad v(200) = -0.039$ (Ry)

This gives

Al: $\beta_2 = 0.6707 \qquad \beta_3 = 0.4430$

Pb: $\beta_2 = 0.5229 \qquad \beta_3 = 0.9079$

The parameter β_1 is obtained from the well known boundary condition for local pseudopotentials

$$\lim \langle \vec{k} + \vec{q}\, |v|\, \vec{k} \rangle = -\frac{2}{3} E_{F_0}. \tag{2}$$

In our case this means

$$\beta_1 \beta_2 = -\frac{2}{3} E_{F_0}, \tag{3}$$

where E_{F_0} is the free electron Fermi level.

2. *Band structure and resistivity of a liquid metal*

The band structure is obtained by solving the secular equation

$$\det |\{(k-g)^2 - E(k)\}\, \delta_{gg'} + S(\vec{g} - \vec{g}')\, \langle \vec{k} + \vec{g}\, |v|\, \vec{k} + \vec{g}' \rangle| = 0. \tag{4}$$

In equation (4) $E(k)$ is the energy, $\vec{g}$ and $\vec{g}'$ are reciprocal lattice vectors and $S(\vec{g} - \vec{g}')$ is the geometrical factor of a face centered cubic lattice. The form of the pseudopotential $\langle \vec{k} + \vec{g}\, |v|\, \vec{k} + \vec{g}' \rangle$ in the secular equation (4) is given by the equation (1). The solution of the secular equation (4) of the order 30 × 30, is obtained with an accuracy of about 0.001 Ry at the corner points

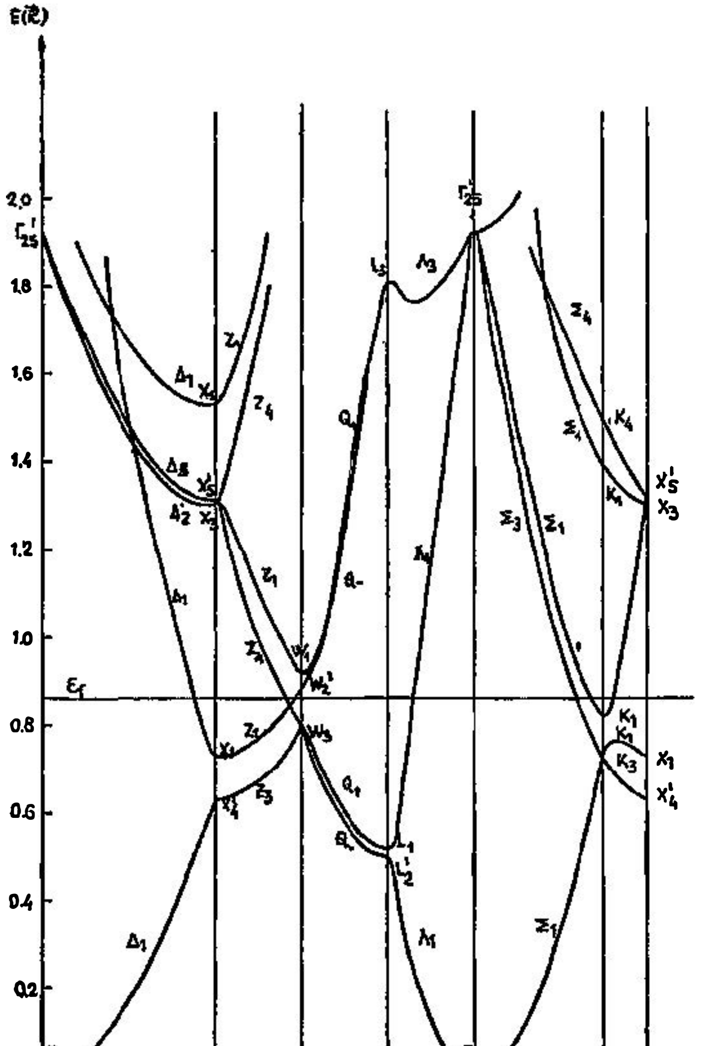

Fig. 1. Energy band of aluminium.

of the Brillouin zone. Obtained results are given in Tables 1 and 2, together with the results of other authors, as well as in figures 1 and 2. The value of the Fermi energy E_F given in tables is obtained according to Ref. 7.

$$E_F = E_{F_0} - \Sigma\, |v(g)|^2\, |S(g)|^2\, (8E_{F_0})^{-1}\, y^{-1} \ln \left| \frac{1+y}{1-y} \right|, \tag{5}$$

where $y = \dfrac{g}{2k_F}$.

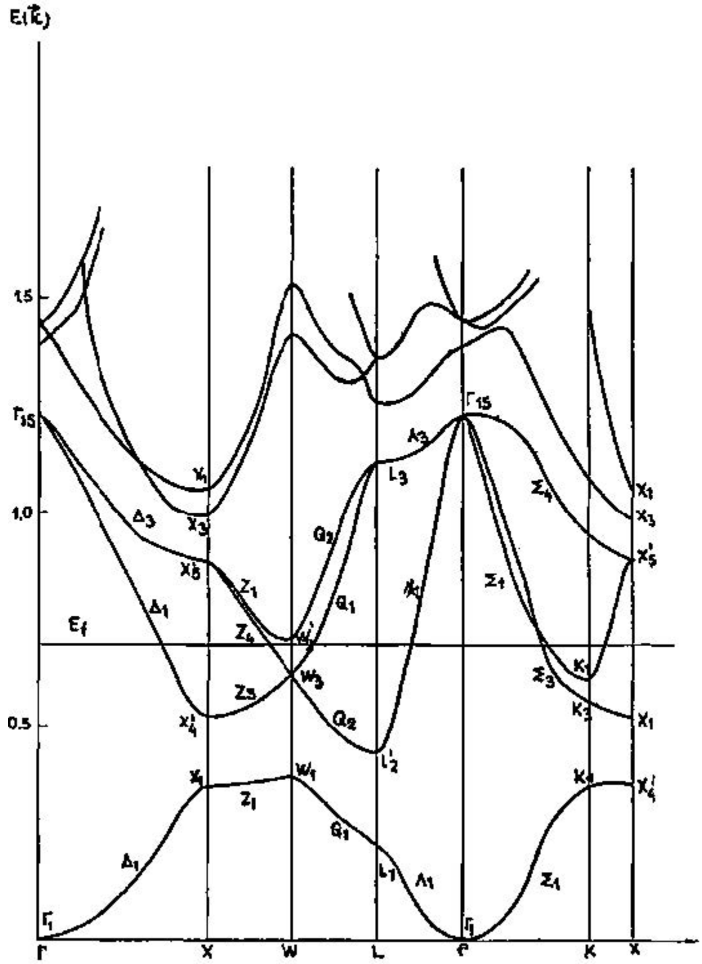

Fig. 2. Energy band of lead.

Our theoretical band structure results for high symmetry points are in a very good agreement with the experiments for Al[8] and Pb[9]. However, discrete experimental form factors of Ashcroft[7] and Anderson and Gold[9] cannot be used for the calculations of the liquid metal resistivities and other physical quantities, where analytical form factors $v(q)$ are needed. On the basis of the pseudopotential (1) proposed in this paper, we have calculated the liquid resistivities of Al and Pb according to the Ziman theory[10]. The results obtained by means of theoretical structure factor and computed from Percus-Yevick equation for a model liquid consisting of hard spheres, are given in Table 3. Theoretical and experimental results are in a good agreement[11].

TABLE 1

	Ashcroft[7]	Pseudopotential (1)
X_4'	0.624	0.628
X_1	0.733	0.728
W_1	0.936	0.916
W_2'	0.873	0.880
W_3	0.793	0.797
L_2'	0.493	0.498
L_1	0.520	0.516
K_3	0.710	0.715
K_1	0.751	0.753
K_1	0.825	0.819
E_F	0.856	0.857

Aluminium. The energy in Ry (1Ry = 13.6 eV) in relation to Γ_1 for some high symmetry points of the Brillouin zone.

TABLE 2

	Anderson and Gold[9]	Pseudopotential (1)
X_1	0.338	0.356
X_4'	0.538	0.518
W_1	0.358	0.380
W_2'	0.724	0.696
W_3	0.647	0.624
L_1	0.239	0.252
L_2'	0.459	0.436
K_1	0.338	0.360
K_3	0.591	0.569
K_1	0.637	0.661
E_F	0.718	0.692

Lead. The energy in Ry (1Ry = 13.6 eV) in relation to Γ_1 for some high symmetry points o the Brillouin zone.

TABLE 3

Metal	T (K)	ϱ_e	ϱ_{SH}
Al	933	24.2	24.5
Pb	673	95	74.5

The resistivity of liquid Al and Pb. ϱ_e is the experimental resistivity at the indicated temperature. Theoretical value is obtained with Sham's[12] dielectric function.

3. *Conclusion*

In conclusion we want to point out that the modification (1) of the general model pseudopotential[1], which supresses the oscillating tail of the form factors in the range of large q-values, gives the satisfactory results for the energy band structure and liquid metal resistivities of typical metals such as Al and Pb.

Acknowledgments

The author is very grateful to S. Zeković, D. Mašović and F. Vukajlović for the interest they took in this work and for their very useful advice.

References

1) V. Veljković and I. Slavić, Phys. Rev. Lett. **29** (1972) 105;
2) V. Veljković, Phys. Letters A **45** (1973) 41;
3) V. Veljković and D. Lalović, Phys. Rev. B **11** (1975) 4242;
4) F. Vukajlović, S. Zeković and V. Veljković, Physica **92** B (1977) 66;
5) M. Blažon, B. Stanojević and V. Veljković, Scripta Met. **1** (1975) 1153;
6) D. Mašović and S. Zeković, Phys. stat. sol. (b) **89** (1978) K57;
7) N. Ashcroft, Phil. Mag. **8** (1963) 2055;
8) I. Weymouth and R. Stedman, Phys. Rev. **B 2** (1970) 4743;
9) I. Anderson and A. Gold, Phys. Rev. **139** (1965) A1459;
10) J. M. Ziman, Phil. Mag. **6** (1961) 1013;
11) N. Ashcroft and J. Lekner, Phys. Rev. **145** (1965) 83.

EFEKAT ODSIJECANJA PSEUDOPOTENCIJALA NA VELIKIM VRIJEDNOSTIMA PROMJENE IMPULSA ZA PRORAČUN ZONSKE STRUKTURE I OTPORA TEČNOG Al I Pb

N. VUKOTIĆ

Nastavnički fakultet, Univerzitet »Veljko Vlahović« 81400 Nikšić

UDK 538.93

Originalni naučni rad

Energetske zone i električni otpor tečnih metala Al i Pb određeni su korištenjem modifikovanog oblika opšteg modelnog pseudopotencijala[1]. Dobiveni rezultati se vrlo dobro slažu sa dobro poznatim rezultatima za ove metale.