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ENERGY BANDS OF POLYVALENT METALS

The general model pseudopotential*) is proposed for simple metals as a function of atomic number. This pseudopotential is successflly applied for the investigations of same features of metals, alloys and intermettallic compounds, and even in the biological systems /2/.

The possibilities of its phenomenological modifications for calculating the band structures of Al and Pb are investigated in this work.

The band structure is obtained by solving the secular equation

$$\det|\{(\vec{k}-\vec{g})^2-\varepsilon(\vec{k})\}\delta_{\vec{g}\vec{g}'}+S(\vec{g}-\vec{g}')<\vec{k}+\vec{g}|v|\vec{k}+\vec{g}'>| = 0 \qquad (1)$$

and $\varepsilon(\vec{k})$ is given in (Ry).

In equation (1) $\vec{g}$ and $\vec{g}'$ are reciprocal lattice vectors and $S(\vec{g}-\vec{g}')$ is the geometrical structure factor of surface centered cubic lattice. $<\vec{k}+\vec{g}|v|\vec{k}+\vec{g}'>$ is formfactor of pseudopotential. The investigations of energy bands have shown that VS pseudopotential does not give satisfactory results for energy bands of Al and Pb, and that is why the modified form of the formfactor of this pseudopotential is suggested in work /6/

$$<\vec{k}+\vec{q}|v|\vec{k}) = S_1\beta_2 j_0(2\pi\beta_2 q/2k_f) + \sum_{i=1}^{2} C_i j_i(2\pi\beta_2 q/2k_f) \qquad (2)$$

The first term in (2) corresponds to the VS pseudopotential. Its parameters β_1 and β_2 are given in the table in the reference /1/, and they are connected by the following relation:

$$\beta_1\beta_2 = -\frac{2}{3}\varepsilon_{fo} \qquad (3)$$

*) We are going to mark Veljković and Slavić's general model pseudopotential with VS.

where ε_{fo} is Fermi level of energy for free electrons. j_0,j_1 and j_2 are spherical Bassel functions of zero, first and second order and C_1 and C_2 are determined by using experimental values for Al and Pb /3,4/

Al: v(111) = 0.0179 (Ry) v(200) = 0.0562 (Ry)

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

This gives

Al: C_1 = 0.18033 (Ry) C_2 = -0.27287 (Ry)

Pb: C_1 = 0.24276 (Ry) C_2 = -0.34881 (Ry)

The proposed modification damps formfactors in area of great q values (Fig.1-2), where they are usually considered as equal to zero /5/.

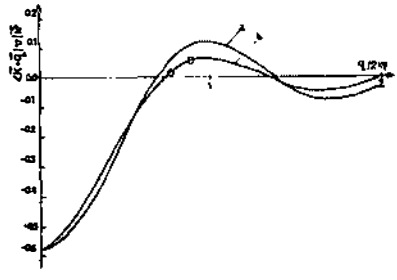

Fig.1. Formfactor Al:
(a) VS pseudopotential
(b) Pseudopotential (2)

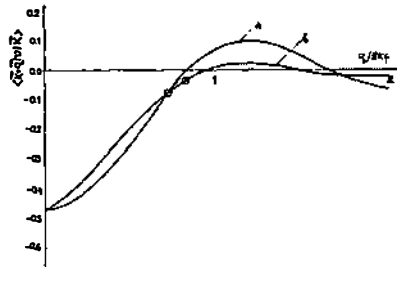

Fig.2. Formfactor Pb:
(a) VS pseudopotential
(b) Pseudopotential (2)

The energy bands of Al and Pb are shown in Fig.3-4. The solution of the secular equation (1) of order 30 x 30, by using (2), is obtained with accuracy of about +0.001 Ry in corner points.

The electronic states in W point of Al (Fig.3) turn out to be the most sensitive to the changes of potentials. The distribution of these states and their relations to the Fermi level show especially good agreement of our results with Ashcroft's model /3/.

The energy band of Pb which the pseudopotential (2) gives shows the regular distribution of energy levels in a valence and conduction band. The level W_3 is double degenerated and it lies beneath Fermi level. This is in accordance with the results of experimental investigations by phenomenological pseudopotential with two parameters /4/. The spin-orbit coupling has not been taken into consideration.

The VS pseudopotential is completed by this suggested modification with two parameters calculated in a very simple and effective way. The obtained results are in good accordance with very well known models of Ashcroft and Anderson-Gold, and with the results of the latest ecperimental investigations. It would be very interesting to investigate its possibilities for calculating some other electronic features of Al and Pb.

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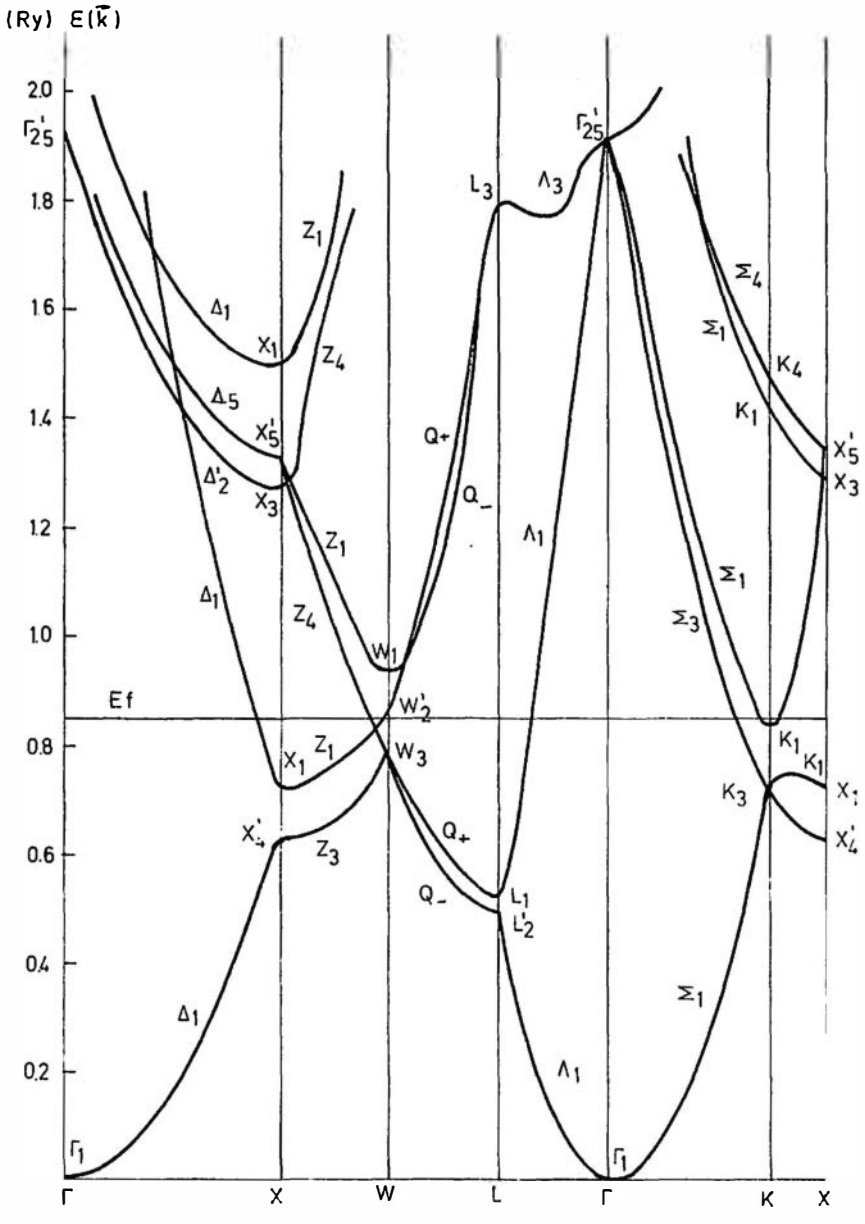

Fig. 3 Energy band of Al

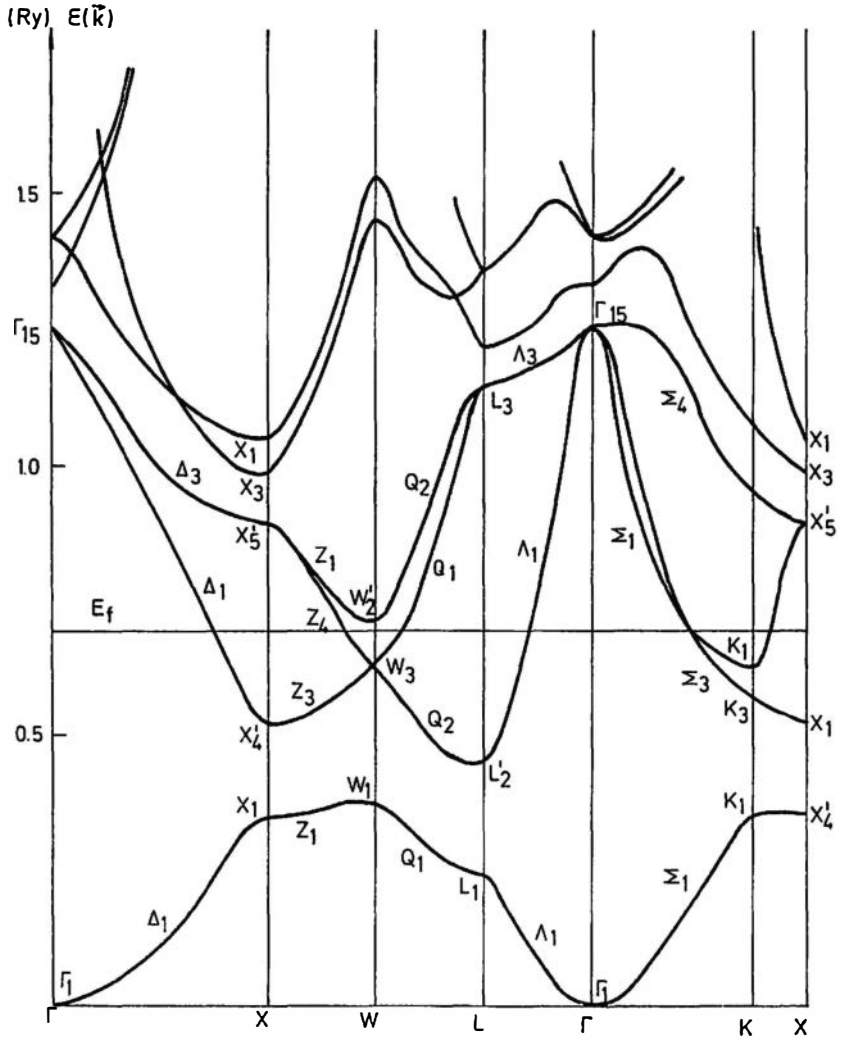

Fig. 4 Energy band of Pb