F I Z I K A V O L U M E 10 S U P P L E M E N T 2, 1978
Proceedings of the VI Yugoslav Symposium of the Physics
of Condensed Matter, Kruševac, September, 18-22, 1978

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MODIFIED VELJKOVIĆ AND SLAVIĆ'S MODEL PSEUDOPOTENTIAL FOR Si, Ge AND Sn

The possibilities of the phenomenological correction of the VS pseudopotential*) /1/ are investigated in the reference /2/ by means of very well known experimental formfactors of Cohen-Bergstresser and Brust /3,4/. This idea is developed in this work like a general procedure for fitting pseudopotential to the experimental values of transition energies in the given crystal.

The band structure of the elementary semiconductors can be obtained by solving the secular equation:

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

where $\varepsilon(\vec{k})$ is in (Ry). In the equation (1), $\vec{g}$ and $\vec{g}'$ are vectors of the reciprocal lattice, while $S(\vec{g}-\vec{g}')$ is the geometrical structure factor of the lattice with a diamond crystal structure. $<\vec{k}+\vec{g}|v|\vec{k}+\vec{g}'>$ is the formfactor of the pseudopotential.

The results for the energy bands of Si, Ge and Sn**) obtained by the VS pseudopotential are completely useless, especially for extremely sensitive energy levels of Γ_2' type which affect a lot electronic features of these materials. That is why we suggest, for calculating the energy band, the modified formfactor of the VS pseudopotential

$$<\vec{k}+\vec{q}|v|\vec{k}> = \beta_1\beta_2 j_0(2\pi\beta_2 q/2k_f) + \sum_{i=1}^{3} C_i j_i(2\pi\beta_2 q/2k_f) \qquad (2)$$

The first term in (2) corresponds to VS pseudopotential. Its parameters are shown in the table in the reference /1/. j_0, j_1, j_2 and j_3 are spherical Bassel's functions of zero, first, second and third order.

The unknown constants C_1, C_2 and C_3 in (2) are determined by fitting the

*) We are going to mark Veljković and Slavić's general model pseudopotential with VS, and its modified version with mVS.

**) α- modification

solution of the equation (1) to the experimental values of transition energies of the given semiconductor.

The algoritham of the method consists of the following blocks:

1. Input data: 1a) formfactors of some very well known phenomenological pseudopotential that gives a "good" energy band, and 1b) limits of reliability of the solution of the equation (1) with reference to the experimental data.

2. For solving the equation (1) we apply Brust´s modification of Löwdin´s perturbation technique /4/ with the parameters N and r chosen in that way so that the divergence of the solution of the equation (1) does not bring about changes beyond the determined limits of reliability.

3. The initial values of constants C_1, C_2 and C_3 in (2) are calculated so that the mVS pseudopotential goes through input phenomenological formfactors.

4. The phenomenological formfactor, to whose changes the energy band is optimally sensitive, is determined. The others are fixed.

5. The value of the optimal formfactor changes at the last decimal with an arbitrary step and we calculate constants of mVS which now goes through new points. We look for the step which causes changes in the energy band within the limits of reliability. If we state that such a step does not exist, we move to the next decimal and the whole procedure is repeated until we obtain it at some decimal. Finally, we investigate the results and determine the formfactor which is most suitable for the experiment.

Results. In /5/ it is mentioned that the limit of accuracy of the experimental transition energies, obtained from the optical and photoemission spectras, is ±0.05eV. By choosing Löwdin´s parameters N=50 and r=89, we provide the convergence of the solution of the equation (1) within allowed experimental accuracy +0.01eV. The formfactors of Cohen-Bergstresser are taken as input data in 1a). By changing the optimal formfactor v(220), we determine constants of mVS in Tab.1. The other two formfactors: v(111) and v(311) have fixed values given in the ref./3/.

The transition energies for Si, Ge and Sn, are shown in Tab.2, compared

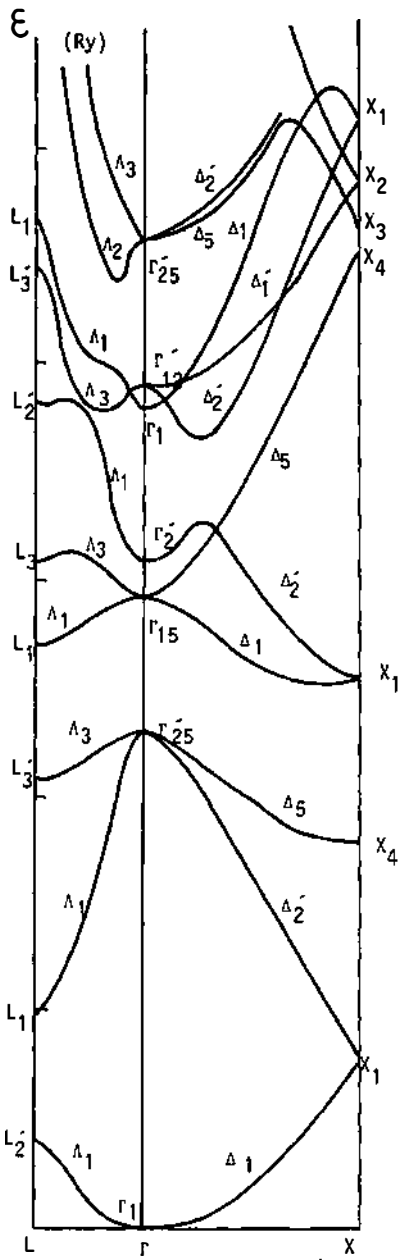

Fig.1 Energy band of Si

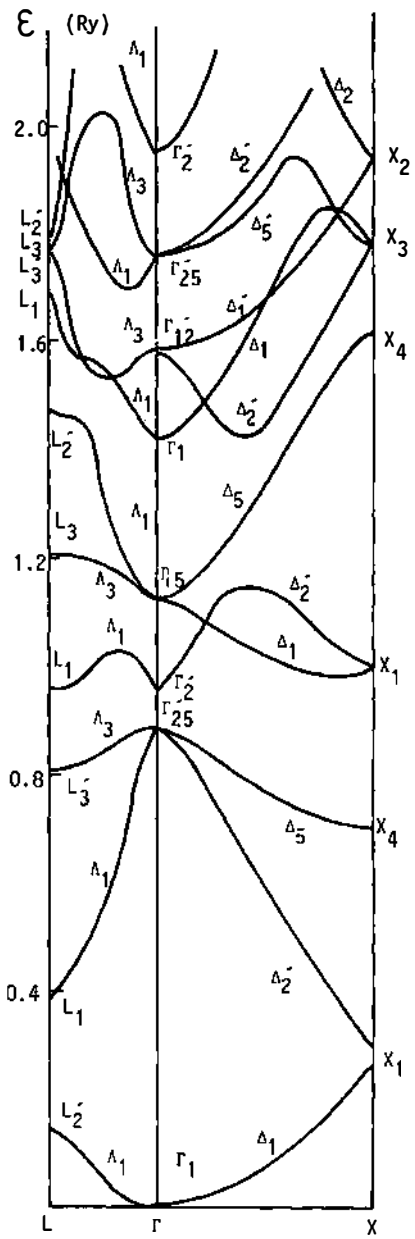

Fig.2 Energy band of Ge

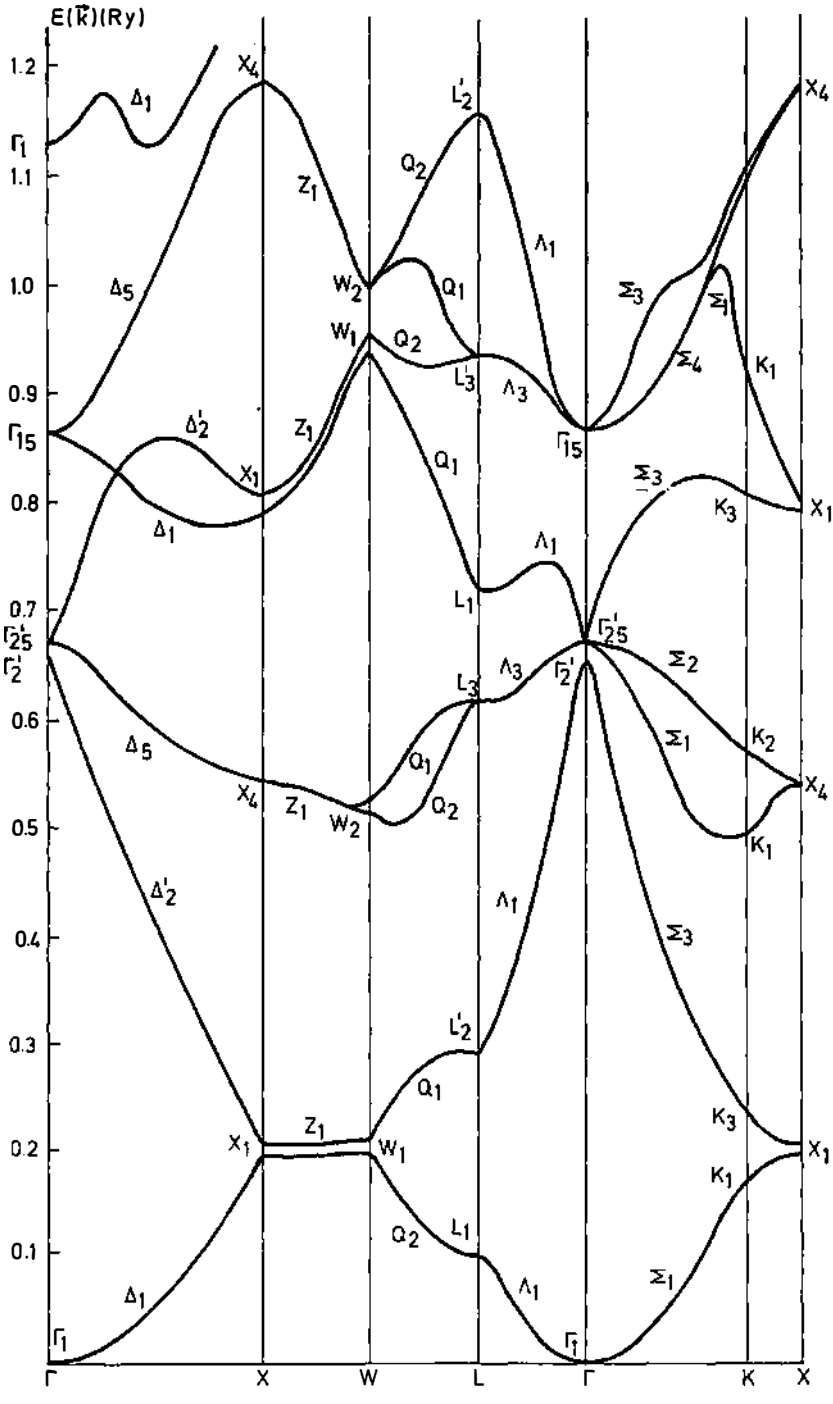

Fig. Energy band of Sn

with the experimental data. Their energy bands are shown in Fig. 1-3. The authors were not able to indentify levels in the higher conduction band between the points Γ-K and W-L of the first Brillouin's zone because they lacked both information and sufficient number of points in $\vec{k}$ space for which $\mathcal{E}(\vec{k})$ was calculated. That is why they only give energy bands for Si and Ge along the direction [100] and [1/2 1/2 1/2]. For the same reason, the whole higher conduction band is left out in the band structure of Sn, calculated along all the characteristic directions of the first Brillouin's zone.

Tab.1. The optimal value and accuracy of the formfactor v(220) for Si,Ge and Sn. The values of C_1,C_2 and C_3 are obtained from the condition that the mVS goes through the points: v(111),v(220) and v(311). All the data are in (Ry).

	Si	Ge	Sn
v(220)	0.0390	0.0000	-0.0120
accuracy	0.0005	0.0005	0.0005
C_1	0.1475	0.2035	0.2600
C_2	-0.3490	-0.6803	-0.6285
C_3	0.1029	0.3914	0.3803

Tab.2. The transition energies for Si, Ge and Sn (eV)

	Si		Ge		Sn	
	mVS	exp./6,7/	mVS	exp./5/	mVS	exp./3,8/
$\Gamma_2'-\Gamma_{25}'$	4.15	4.15	0.97	0.99	-0.20	-0.16
$\Gamma_{15}-\Gamma_{25}'$	3.35	3.45	3.18	3.23	2.60	2.9
$L_1-\Gamma_{25}'$	2.07	-	1.00	0.84	0.68	0.32
$X_1(\Delta_1)-\Gamma_{25}'$	-	-	1.49	1.26	1.60	-
L_1-L_3'	3.31	3.40	2.19	2.34	1.39	1.4
L_3-L_3'	5.41	5.1	5.39	5.80	4.33	4.4
X_1-X_4	4.12	4.30	3.98	4.50	3.29	3.5

The results for energy transition obtained by mVs pseudopotential are more precise and in a better agreement with experimental data than very well known Cohen and Bergstresser's results, esspecialy for very important transition around band gap: $\Gamma_2'-\Gamma_{25}'$, L_1-L_3' and X_1-X_4. This pseudopotential has been tested by calculating the resistivities in the liquid phase of Si, Ge and Sn, whereas obtained results will be presented in one of the following works.

Acknowledgements. The authors are very thenkful to Dr Filip Vukajlović and Dr Veljko Veljković for the interest they had in this work and for very useful advices.

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