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Application of the Lattice Model to Semiconductors of the Lead Sulphide Type

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THE application of the lattice model to solids was first pointed out by Coulson[1], who calculated (with the aid of this model) the band structure of the energy spectrum in metals with a cubic space lattice, and also in graphite and in boron nitride. In the present paper the lattice model is applied to semiconductors of the type PbX, where X = S, Se and Te. The specified semiconductors have cubic lattices of the NaCl type. The initial electron configurations in the isolated atoms are: Pb$-p^2$, $X-p^4$. For each of the paired atoms of PbX in the crystal there are six p-electrons. We may consider two lattice models of PbX crystals:

a) the three-dimensional model, analogous to the three-dimensional lattice model, proposed by Coulson for metals;

b) it is possible to describe the p-electrons in the crystal as breaking up into the groups p_x, p_y and p_z, and the electrons of each group break up into subgroups, such that all electrons of one subgroup can move in a definite plane of the tetragonal lattice, formed by the atoms of Pb and X. Each of the subgroups is similar to a system of $\pi-$electrons in conjugate organic molecules.

In the first, as well as in the second model, we set the following for the potential V along the lattice: $V = V_0$ within the Pb atoms and $V = 0$ within the X atoms (V_0 is the difference between the electronegativities of X and Pb). For conjugate organic molecules containing heterocyclic atoms, Veselov and Rekasheva[2] proposed such a form for the potential.

In order to determine the size of the atoms of Pb and X in the crystal, we start out from the value of the ionic radii of Pb^{++} and X^{--} (according to Goldshmidt). The initial values of the ionic radii r_{Pb} and r_X are changed in proportion so that in each crystal the equation $r_{Pb} + r_X = a$ holds (a is the distance between the atoms Pb and X).

We have the following relation for the binding energy of the electron and its quasi-momentum $\mathbf{k}$:

In the first model

$$f(E) = {}^1/_9 (\cos ak_x + \cos ak_y + \cos ak_z)^2;$$

In the second model

$$f(E) = {}^1/_4 (\cos ak_x + \cos ak_y)^2.$$

The function $f(E)$ has the following form:

$$f(E) = (\cos \omega_1 r_X \operatorname{ch} \omega_2 r_{Pb} - (\omega_1/\omega_2) \sin \omega_1 r_X \operatorname{sh} \omega_2 r_{Pb})$$
$$\times (\cos \omega_1 r_X \operatorname{ch} \omega_2 r_{Pb} + (\omega_2/\omega_1) \sin \omega_1 r_X \operatorname{sh} \omega_2 r_{Pb}),$$

if $E < V_0$ and

$$f(E) = (\cos \omega_1 r_X \cos \omega_2 r_{Pb} - (\omega_1/\omega_2) \sin \omega_1 r_X \sin \omega_2 r_{Pb})$$
$$\times (\cos \omega_1 r_X \cos \omega_2 r_{Pb} - (\omega_2/\omega_1) \sin \omega_1 r_X \sin \omega_2 r_{Pb}),$$

$$\omega_1 = \sqrt{2E};\ \omega_2 = \sqrt{2|E - V|},$$

if $E > V_0$. The allowed energy values in the first and second models are determined from the equation

$$0 \leqslant f(E) \leqslant 1.$$

In this manner the three-dimensional and the plane model lead to the same band structure for the energy spectrum. At absolute zero, the first allowed band in the first as well as in the second model is completely filled with electrons, the remaining allowed zones are empty.

We calculated the width of the forbidden zone ΔE, the effective mass of the holes m_h^* and the effective mass of the electrons m_e^* (in units of the

electronic mass) in the semiconductors under consideration:

	r_{Pb}, Å	r_X, Å	V_0, eV	ΔE, eV	$\Delta E/\Delta E^{(1)}_{exp}$	$\Delta E/\Delta E^{(2)}_{exp}$	m^*_h	m^*_e
PbS	1.28	1.68	2.50	1.48	1.42	1.06	2.03	1.02
PbSe	1.25	1.82	1.95	1.13	1.36	1.08	1.54	0.88
PbTe	1.22	1.95	1.39	0.79	1.27	0.88	1.07	0.70

There are presented in the Table the values of the effective mass corresponding to the second model. The values which correspond to the first model can be derived by multiplying them by 2.25. The experimental values of the widths of the forbidden zones $\Delta E^{(1)}_{exp}$ are taken from Ref. 3, $\Delta^{(2)}_{exp}$ from Ref. 4. The value of V_0 was taken from Ref. 5. Notice that the derived value of ΔE, and also the values of the effective mass, may change somewhat, owing to some uncertainty in the values of the parameters r_{Pb}, r_X and V_0. Nevertheless, we think that the results obtained confirm the applicability of the lattice model to semiconductors and the desirability of extending its applications in this direction.

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Photoproduction of π–Meson Pairs in Hydrogen and Deuterium Near Threshold and Isotopic Invariance

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THE cross section for photoproduction of π–meson pairs in hydrogen and deuterium is calculated by considering the interaction of an electromagnetic field with a meson-nucleon system in first order perturbation theory (it is well known that this does not presuppose a small interaction between mesons and nucleons). The interaction operator consists of two parts[1] $H = S + V_3$, where S is a scalar and V_3, the third component of a vector is isotopic spin space.

The isotopic spin of the initial state in the reaction

$$\gamma + p \to n' + \pi' + \pi'' \qquad (1)$$

is equal to ½. The isotopic spin of the meson-nucleon system in the final state may be $t = ½$ and $t = 3/2$. The operator S yields transitions to states of the meson-nucleon system with isotopic spin $t = ½$, and the operator V_3 to states $t = ½$ and $t = 3/2$.

S_{Tt} V_{Tt} will be used to denote transition amplitudes to states of total isotopic spins $t = ½$ and 3/2 of the meson-nucleon system, and isotopic spin T of the two π–mesons system ($T = 0, 1, 2$). The differential cross section for photoproduction of two π–mesons then becomes

$$\sigma_1(\gamma + p \to p + \pi^0 + \pi^0) \qquad (2)$$

$$= \left| \frac{1}{\sqrt{3}} S_{0^1/_2} + \frac{1}{3} V_{0^1/_2} + \frac{2}{3}\sqrt{\frac{2}{5}} V_{2^2/_2} \right|^2;$$

$$\sigma_2(\gamma + p \to p + \pi^+ + \pi^-)$$

$$= \left| \frac{1}{\sqrt{3}} S_{0^1/_2} + \frac{1}{3} V_{0^1/_2} - \frac{1}{3}\sqrt{\frac{2}{5}} V_{2_{3/_2}} \right.$$

$$\left. + \frac{1}{\sqrt{6}} S_{1^1/_2} + \frac{1}{3\sqrt{2}} V_{1^1/_2} - \frac{\sqrt{2}}{3} V_{1^2/_2} \right|^2; \qquad (3)$$