DEPENDENCE OF THE NATURE OF THE ELECTRON ENERGY BANDS IN A SEMICONDUCTING FILM ON ITS THICKNESS

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A group-theoretical method is given for considering the band structure of crystalline films. This method is applied to determine the nature of the splitting of the valence band edge in Ge and Si films.

THE symmetry of a crystal leads to the degeneracy of the electron energy levels in the crystal—to the merging of bands at singular points of a Brillouin zone. Thus, because of the cubic symmetry, the valence band edge in Ge and Si is triply degenerate.[1] (This corresponds to $k = 0$ and the F_1 representation of the O_h group; the notation of the representation follows [2].) The degeneracy is partly lifted by the spin-orbit interaction. Two levels appear, corresponding to the extra-representations of the double group O_h.

In the case of a semiconducting film, its finite thickness (i.e. its "boundedness") along one dimension should have an effect. The present note attempts to determine the influence of this "boundedness" on the nature of the splitting of the energy bands.

The presence of boundaries in a film reduces the symmetry, which no longer represents a Fedorov group but is one of the 80 groups of the two-dimensional lattice. Also, a crystalline film consists of many atomic layers. Therefore, the state of being a film is manifest as a small perturbation. Consequently, the influence of the "boundedness" may, by reducing the symmetry, lift the degeneracy partly or completely. In the case of the valence band edge of Ge or Si, the "boundedness" of the film must lift the threefold degeneracy (without allowance for the spin-orbit interaction), since the planar groups have no three-dimensional irreducible representations corresponding to $k = 0$. In particular, if the normal to the film is oriented along [111], the zeroth wave vector group is D_{3d} and there is splitting into two levels: $F_1 = A_2 + E$.

The order of magnitude of the splitting may be regarded as roughly equal to the ratio of the band width and the number of atomic layers in the film. For films 10^{-6} cm thick, such an estimate gives tenths of an electron-volt. We can estimate this splitting from the uncertainty principle. For the usual film thicknesses ($\approx 10^{-6}$ cm), $\Delta E \sim h^2k^2/2m \sim 10^{-12}$ erg, i.e., it is of the same order. Obviously, the splitting due to the "boundedness" of the film increases as the film gets thinner.

These estimates of the magnitude of the splitting cannot, of course, be expected to give quantitative agreement with reality. However, it follows from them that it should be possible to determine experimentally the splitting of the levels due to the finite thickness of the film.

We have not allowed for the spin-orbit splitting.[3] In principle, it may be smaller or greater than the splitting due to the finite film thickness. In the former case, the spin-orbit interaction should be regarded as a small perturbation of the levels obtained by allowing for the finite film thickness. For Si and Ge, this leads to an additional splitting of the doublet: $A_2 \rightarrow E_2'$, $E \rightarrow E_1' + E_2'$.

In the case when the spin-orbit interaction is more important than the perturbation due to the finite thickness of the film, the nature of the splitting is found by expanding the extra-representation of a Fedorov group in terms of irreducible extra-representations of the double group of the two-dimensional space symmetry. Since all the extra-representations of these groups are nondegenerate (without allowance for the twofold Kramers degeneracy), the finite thickness of the film may also lead to complete splitting of the valence-band edge in Si and Ge into three levels.

[1] F. Herman, Revs. Modern Phys. **30**, 102 (1958).

[2] L. Landau and E. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, 1963.

[3] L. Huldt and T. Staflin, Phys. Rev. Letters **1**, 236, 313 (1958).

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