Vasileff's Calculation of Electronic Self-Energy in Semiconductors

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It is shown that Vasileff's theory expressing the shift of the thermal band edge in terms of such parameters as effective mass fails for semiconductors of the usual type because of the predominance of processes involving virtual phonons of large wave number.

VASILEFF[1] has recently given a theory of the change with temperature of the electronic energy gap and carrier effective mass. He has applied the theory to the semiconductors germanium and silicon. His theory suggests that there is a relation among the three quantities: the temperature variation of the energy gap, the coupling constant for scattering, and the effective mass.

The purpose of this note is to point out that Vasileff's model fails, and that as a consequence his formula does not apply to any of the familiar semiconductors.

Following Fan,[2] Vasileff assumes that the shift with temperature of the energy gap results from what are sometimes referred to as virtual absorption and emission of phonons by electrons. Vasileff uses the deformable potential theory of the electron-phonon interaction and assumes that the important virtual processes involve phonons of wave number small compared to the reciprocal lattice spacing.

Now it can readily be seen that in fact the virtual processes of large wave number are the important ones in giving the energy-gap shift. Thus Vasileff's Eqs. (5.1)–(5.3), evaluated at $\Delta k=0$, show that the shift is proportional to an integral which depends on wave number like

$$\int_0^{\sigma_m} \sigma d\sigma (N_\sigma+\tfrac{1}{2}), \qquad (1)$$

where N_σ is the phonon occupation number for the mode σ, and σ_m is the maximum phonon number. At high temperatures $N_\sigma+\frac{1}{2}$ may be replaced by $KT/\hbar\sigma s_\sigma$, where s_σ is the phonon velocity and K is Boltzmann's constant; and the integral (1) gives a linear dependence on T as given by Fan.[2] Clearly, the relative contributions to the integral (1) of different wave number intervals is such that "in σ space, shells of equal thickness make equal contributions." Consequently most of the integral is contributed by processes of large wave number. At large wave number it is certain that the effective mass approximation and the deformable potential model both fail.

That there is an approximate quadratic dependence of the shift on temperature at low temperatures as found by Vasileff is not surprising and does not depend in a detailed way on the assumptions he made. A quadratic temperature dependence requires only that shells of equal thickness in σ space contribute about equally to the energy gap shift. Then, since below the Debye temperature the modes that have $N_\sigma \gtrsim 1$ will all be modes for which $\hbar\sigma s_\sigma < KT$, the integral (1) would have to be broken into two parts, an integral over modes in zero-point vibration and an integral over modes that are vibrating approximately classically. It is easily shown by even a very crude calculation that this must give for the energy-gap shift an approximate quadratic dependence on T below the Debye temperature.

It would be very surprising if the calculation of Vasileff gave an even roughly correct result in a semiconductor for which the effective mass is small, because in such a case the small mass will result in a considerable overestimate of the average energy denominators for the virtual processes. For germanium, with $m_{\text{eff}} \sim 0.1 m_0$, this formula could underestimate the shift by an order of magnitude.

The objections raised against the application to germanium should be valid for application to almost any other semiconductor. We doubt that in general a quantitative interpretation of the energy gap shift will prove feasible on the basis of a fundamental theory such as that of Vasileff, because of the expected predominance of the large-phonon processes.

[1] H. D. Vasileff, Phys. Rev. **105**, 441 (1957).
[2] H. Y. Fan, Phys. Rev. **82**, 900 (1951).