

Concerning impuriton diffusion in solid H⁴

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As is well known,^[1,2] the diffusion of point defect in quantum crystals at low temperatures reduces to diffusion of corresponding quasiparticles—defectons. It was shown in^[2-4] that the coefficient of diffusion of defectons in a phonon gas is given by

$$D_{\text{ph}} = 20 \frac{ac}{\sigma_0} \left(\frac{\epsilon}{\theta} \right)^2 \left(\frac{\theta}{8T} \right)^9, \quad (1)$$

and the free path time is

$$\tau = 7.8 \frac{\tau_0}{\sigma_0} \frac{\epsilon}{\theta} \left(\frac{\theta}{8T} \right)^9, \quad (2)$$

where a is the lattice constant, c is the speed of sound, θ is the Debye temperature, $\tau_0 = \hbar/A$ is the defect delocalization time, A is the amplitude of the probability of the tunnel transition of the defect to the neighboring site, ϵ is the width of the defecton band, and σ_0 is a constant connected with the change of the dynamic matrix around the defect. In the case of a vacancy we have $\sigma_0 = 1$, and in the case of an isotopic impurity we have $\sigma_0 = [(M-m)/M]^2$ (m and M are the masses of the lattice atom and of the defect, respectively).

Formulas (1) and (2) are valid at temperatures that are high in comparison with the width of the band ($T > \epsilon$). However, in order for the defectons to be good quasiparticles, it is necessary that the free path time be larger than the defect-delocalization time. Consequently, quantum diffusion should be observed at temperatures below a certain characteristic temperature T^* , which is determined from (2):

$$T^* = \frac{\theta}{8} \left(\frac{7.8 \epsilon}{\sigma_0 \theta} \right)^{1/9}. \quad (3)$$

Thus, with decreasing temperature, a rapid growth of the diffusion coefficient should be observed. Its natural upper limit is imposed by the interaction between the defects.

If we denote by σ the cross section for the scattering of a defecton by a defecton (in units of a^2), then we can show that at absolute zero temperature and at a given concentration x of the defects the diffusion coefficient will be

$$D_0 = \frac{ac}{zx\sigma} \frac{\epsilon}{\theta}, \quad (4)$$

where Z is the number of nearest neighbors, and the mean free path is

$$l = \frac{a}{\sqrt{2}zx}. \quad (5)$$

If the phonon and defecton mechanisms are assumed to be independent, then the total diffusion coefficient D can be written in the form

$$D^{-1} = D_0^{-1} + D_{\text{ph}}^{-1} = \frac{1}{ac} \frac{\theta}{\epsilon} \left\{ zx\sigma + \frac{\sigma_0}{20} \frac{\theta}{\epsilon} \left(\frac{8T}{\theta} \right)^9 \right\}. \quad (6)$$

A similar interpolation formula was used in^[5,6] for the reduction of the experimental data on the diffusion of He³ impurities in solid He⁴. Notice should be taken, however, of certain essential differences. In (6) the characteristic temperature is not θ , but $\theta/8$, a very important difference, since this quantity is raised to the ninth power. Another feature is connected with the cross section σ for the scattering of defects by defectons. As shown in^[2], in view of the small width of the defecton band, σ can turn out to be anomalously large. Thus, e. g., in the case of isotropic interaction $U(r) = V_0(a/r)^6$, we have

$$\sigma \approx 2\pi \left(z \frac{V_0}{\epsilon} \right)^{2/5}. \quad (7)$$

Thus, the concentrations at which the defects can be regarded as noninteracting is determined from the condition $l \gg a$, i. e.,

$$x < \frac{1}{\sigma} \sim \left(z \frac{\epsilon}{V_0} \right)^{2/5}. \quad (8)$$

Let us estimate the width of the defecton band, using the experimental results^[5-7]

$$D_0 x = (1.2 \pm 0.4) 10^{-11} \text{ cm}^2/\text{sec}, \quad (9)$$

$$D_{\text{ph}}^{-1} = 4.6 \cdot 10^6 T^6, \quad (10)$$

$$\theta = 26^\circ\text{K}, \quad a = 4 \cdot 10^{-8} \text{ cm}, \quad c = 5 \cdot 10^4 \text{ cm/sec.}$$

Comparing (10) and (1) we obtain $\epsilon \approx 10^{-4}$ deg, and from (4) and (9) we determine the order of magnitude of the scattering cross section, $\sigma \approx 6 \times 10^2$.

Substituting this value in (8), we see that the concentration at which one can observe the defecton diffusion mechanism should satisfy the inequality $x < 2 \times 10^{-3}$. It is therefore not surprising that no quantum diffusion was observed in^[8] down to 0.4 °K, since the experiment was carried out at concentrations $x = 7.5 \times 10^{-3}$.

Calculation of the characteristic temperature T^* from formula (3) yields $T^* = 1.3$ °K, which is also in good agreement with experiment.^[5]

Let us return finally to formula (7). If we assume that in order of magnitude $V_0 \sim \Delta mc^2/2$, then we obtain from (7) that $\sigma \approx 10^3$.

We see thus that the proposed theory is self-consistent and shows good agreement with the experimental results. We note also that the value calculated by us for the width of the defecton band is larger by approximately two orders of magnitude than that obtained in^[5]. This is apparently due to the inaccuracy of the interpolation

formula used in that reference and to failure to take into account the large cross section for scattering of the defecton by a defecton.

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Formula (10) on p. 386 should read $D_{ph}^{-1} = 4.6 \times 10^6 T^9$.