Effect of vacancions on a crystal lattice structure

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It is shown that under certain conditions the delocalization of a vacancy in a quantum crystal should be accompanied by a local phase stratification and by the formation of an impurity-free region.

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The transformation of a point defect (vacancy, impurity, etc.) into a defecton (vacancion, impuriton, etc.) in an ideal crystal is connected with a decrease of the crystal energy.[1,2] The bottom of the defecton band lies lower than the energy of the crystal with the localized defect, by an amount equal to the half-width of the defecton band. If the half-width of the band turns out to be larger than the activation energy of the defect (null/defectons), then this should lead to a restructuring of the ground state of the crystal.[1] However, as will be shown below, even if the band width ϵ is less than the activation energy, the presence of defectons can substantially influence the

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configuration of the lattice atoms. As a result, the distribution of the impurities around the vacancy can change, and local phase stratification is also possible.

Consider a quantum crystal such as solid helium, which contains a vacancy and isotoptic impurities with dimensionless concentration x. Generally speaking, the energy of such a system depends on the distribution of the impurities and on the environment of the vacancy in the lattice. In the case of low isotopic-impurity concentrations and a localized vacancy, obviously, this dependence can be neglected. The picture changes substantially, however, if account is taken of the fact that for a vacancion to be produced the lattice must have good periodicity. Thus, we can expect a region "free" of impurities to be produced around the vacancy. A similar situation arises in fluctuon formation [3,4] and in the formation of magnetically ordered regions around vacancies in ^{3}He.[5] Since the width of the vacancion band is much larger than the width of the impuriton band, the time within which the vacancion adjusts itself to a given configuration of impurities is much shorter than the time of the change of this configuration. If $T \ll \epsilon$, then the vacancion has a quadratic dispersion and its effective mass is $m^* = \hbar^2/2A$, where A is the probability of the transition of the vacancy to the neighboring site (the lattice constant is $a = 1$). The energy of a vacancion trapped in a region of dimension R can be estimated from the uncertainty relation

$$E = \epsilon_0 + \pi^2 \frac{A}{R^2},$$

where ϵ_0 is the energy of the bottom of the vacancion band. The free energy is then

$$F = E - TS = \epsilon_0 + \pi^2 \frac{A}{R^2} - Ts \frac{4}{3} \pi R^3,$$

where s is the entropy per cell. If the impurity concentration is so small that the impurities can be regarded as an ideal gas, then $s = x \ln(x/e)$, and in the more general case of a "lattice" gas we have

$$s = x \ln x + (1 - x) \ln(1 - x).$$

The dimension of the region "rid" of impurities can be determined from the condition that the free energy be a minimum. We thus obtain

$$R = \left| \frac{\pi A}{2Ts} \right|^{1/5}, \quad F_{min} = \epsilon_0 + \frac{10\pi}{3} \left(\frac{\pi A}{2} \right)^{3/5} T^{2/5} |s|^{2/5}.$$

The condition for the applicability of this relation is the inequality $R \gg 1$, i.e., $A \gg |Ts|$, which is ensured by the condition of the use of the effective mass. Thus, the presence of vacancions should stimulate stratification of He^3–He^4 solutions. On the other hand, the presence of impurities influences the equilibrium vacancy concentration $|n_v|$. In fact

$$n_v \sim e^{-\frac{F}{T}} = \exp\left\{ -\frac{\epsilon_0}{T} - \frac{10\pi}{3} \left(\frac{\pi A}{2T} \right)^{3/5} |s|^{2/5} \right\}.$$

The presence of vacancions can cause also local phase stratification if the widths of the vacancion bands in the two phases differ greatly and the heat of the transition is small. Such a situation arises apparently for the two He^4 phases (hcp and bcc). As shown in [6], the width of the vacancion band depends exponentially on the number of nearest neighbors and should consequently change strongly on going from one phase to another. If a new phase is produced in a region of dimension R around the vacancy, then the change of the free energy is

$$\Delta F = \Delta\epsilon_0 + \frac{\pi^2 A}{R^2} - T\Delta s \frac{4}{3}\pi R^3,$$

where $\Delta\epsilon_0$ is the shift of the bottom of the vacancion band and Δs is the difference between the entropies of the two phases. Recognizing that $T\Delta s$ is equal to the heat of transition q, we obtain

$$R = (\pi A/2q)^{1/3}.$$

Since the heat of transition per particle is $q \sim 10^{-2}$ K, and the width of the band is of the order of 10 K, there are $\sim 10^2$ atoms in the volume of the new phase. Of course, this can strongly influence the vacancy mobility, which will now be determined by the kinetics of the phase transition.

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