On the low-temperature maximum of thermal conductivity in cryocrystals

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Abstract

A model of quantum p excitations of atoms in cryocrystals is used to describe the observed low-temperature maximum of the thermal conductivity.

Key words: cryocrystals; delocalized excitations; quantum transitions; heat conductivity

At low temperatures, atoms in a condensed matter can exhibit quantum properties. A well-known example of such behavior is a tunneling transition of atoms in a two-well potential, leading to a fractional-power temperature dependence of the heat capacity of glasses [1]. An atom in a crystal, located in an averaged potential of neighboring atoms, can also undergo quantum transitions from the ground s state to a first excited p state in its own potential well [2,3]. Such a transition is initiated by interaction of atoms with the phonon modes [4] and results in absorption of energy by the atom and modification of the character of distribution of quantum displacements of the excited atom near a site of the crystal lattice. Due to both translational symmetry of the crystal and inductive interactions of the atom in the p state with neighboring non-excited atoms, this p excitation propagates through the crystal by a wide enough p band, whose bottom is separated from the s state energy level by a gap E_g. For example, $E_g \sim 5-6$ K in ^{4}He crystals [2–4], $E_g \sim 20-25$ K in solid Ne, Ar, Kr and Xe [5]. The effective mass of an excitation is small and represents about 10 percent of the atomic mass [4,5]. An effective radius of an excited atom of the crystal is somewhat larger than that of an atom in the s state, so that one can consider a p excitation as a delocalized point defect of the crystal, which has an excess energy and is able to transfer the energy through the crystal.

To estimate a low temperature contribution of the p excitations to the crystal heat conductivity, one can treat them as a gas of particles, whose free path λ is determined by their interactions with the long-wave phonon modes. In such representation, invoking results of the the kinetic theory of gases, we express the coefficient K_p of the heat conductivity as

$$K_p = \frac{1}{3}\frac{C_V}{V}\, v\lambda, \tag{1}$$

where C_V is the isochoric heat capacity of the gas of p excitations, V is its volume, v is average velocity of a particle, transferring the energy. As follows from the quantum diffusion theory [6], for wide-band particles at low temperatures,

$$\lambda \sim T^{-7}. \tag{2}$$

The heat capacity of the gas of p excitations is given by [4]

$$C_V = V\left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2} e^{-E_{\rm g}/T} \tag{3}$$

$$\times\left[1 + \frac{5T}{2E_{\rm g}} + \frac{5}{2}\left(\frac{T}{E_{\rm g}}\right)^2\right]. \tag{4}$$

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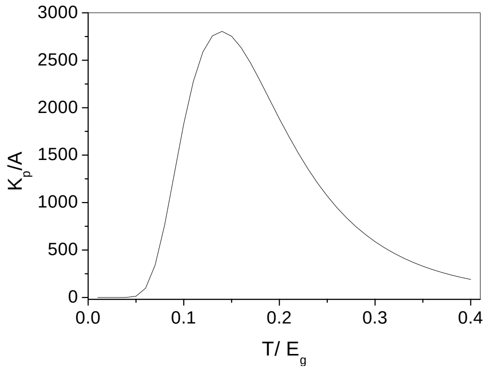

Fig. 1. Reduced thermal conductivity $K_p(T)/A$ versus reduced temperature $T/E_{\rm g}$.

Then the temperature-dependent part of K_p is written as

$$K_p = Ae^{-E_{\rm g}/T}\left(\frac{E_{\rm g}}{T}\right)^{15/2}\left[1+\frac{5T}{2E_{\rm g}}+\frac{5}{2}\left(\frac{T}{E_{\rm g}}\right)^2\right]. (5)$$

In Fig. 1 we present the temperature dependence of the reduced thermal conductivity K_p/A in the low-temperature range. The shape of the $K_p(T)$ curve and the degree of maximal increasing of K_p are in good agreement with the experimental data [7]. The calculated position T_m of the maximum of the $K_p(T)$ dependence is also in good correlation with the observed ones. For example, $T_m \approx 0.2E_{\rm g} \approx 1.2$ K for ^{4}He, $T_m \approx 0.2E_{\rm g} \approx 4$ K for Ar.

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