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On the low-temperature anomalies in the thermal conductivity of plastically deformed crystals due to phonon–kink scattering

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Previous experimental studies of the thermal conductivity of plastically deformed lead crystals in the superconducting state have shown strong anomalies in the thermal conductivity. Similar effects were also found for the thermal conductivity of bent ^{4}He samples. Until now, a theoretical explanation for these results was missing. In this paper we will introduce the process of phonon–kink scattering and show that it qualitatively explains the anomalies that experiments had found.

PACS: **72.10.–d** Theory of electronic transport; scattering mechanisms;
72.15.Eb Electrical and thermal conduction in crystalline metals and alloys;
66.70.–f Nonelectronic thermal conduction and heat-pulse propagation in solids; thermal waves;
61.72.Lk Linear defects: dislocations, disclinations;
67.80.–s Quantum solids.

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1. Introduction

Previous studies of the thermal conductivity of lead crystals in the superconducting state, which were deformed plastically by low-temperature stretching of the initially perfect samples, and observation of the recovery processes on annealing of the samples at room temperatures, had demonstrated strong anomalies in the thermal conductivity of the deformed Pb crystals below 4 K [1]. The same effects were also seen in weakly bent Bi crystals [2]. Furthermore, experiments on the thermal conductivity of hcp ^{4}He crystals grown from high pure ^{4}He in a long capillary had also revealed strong anomalies in thermal conductivity of samples that were weakly deformed by bending them at temperatures near and above 0.4 K [3,4].

Several attempts for a theoretical explanation of these results have been made, but none have unfortunately been completely successful [5]. In this primer paper however, we introduce a new model for explaining the observed anomalies in the thermal conductivity of the weakly deformed crystals from high pure matter. This model is based on phonon scattering on mobile kinks on the newly induced dislocation lines. Previously, a similar model, based on scattering of electrons by mobile kinks, has been introduced for the explanation of the anomaly in the electronic contribution to the thermal conductivity of plastically deformed copper crystals [6]. In systems where the phonon thermal conductivity is the main contribution to the transfer of heat flux, such as quantum crystals, metal crystals in superconducting state and nonmetals, the scattering of thermal phonons by the mobile kinks on dislocation lines induced under weak deformation of initially perfect samples at reduced temperatures seems to be the natural explanation of the experimentally observed effects. This paper will only introduce this process and show the main results of detailed calculations of the thermal conductivity in different directions relative to the glide plane of the dislocations. We have found that in the crystals where scattering of phonons on kinks is the dominant scattering process our theoretical results can qualitatively reproduce the experimental features. The detailed calculations referred to in this primer note and the quantitative fit of the experimental results can be found in a paper which is soon to appear [7].

2. Kinematics

For a description of the kinematics of phonon–kink scattering we use a similar procedure from Ref. 8. We consider a crystal which contains dislocations due to an external influence on the crystal. The dislocations lie in the xz plane and the direction parallel to the dislocations is the z direction.

Around a dislocation the displacement u_j can be decomposed in two components

$$u_j = u_j^s + u_j^d. \quad (1)$$

The "static" displacement u_j^s depends on the presence of the kinks and can be written as

$$u_j^s = \sum_{\kappa} f_j(\mathbf{r}_\perp : \kappa)\xi_0(\kappa)\mathrm{e}^{i\kappa(z-z_0(t))} + u_{j0}^s, \quad (2)$$

where $\xi_0(\kappa)$ is the Fourier transform of the dislocation's line displacement due to the kink, $f_j(\mathbf{r}_\perp : \kappa)$ is a proportionality constant and u_{j0}^s is displacement around the straight dislocation without kink. The abbreviation $\mathbf{r}_\perp$ indicates (x, y). The "dynamical" displacement u_j^d has its origin in the phonons and can be expressed as a superposition of plane waves,

$$u_j^d = \sum_{\mathbf{k},s} q(\mathbf{k},s)e_j(\mathbf{k},s)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}, \quad (3)$$

where s indicates the polarization of the lattice vibrations and $\mathbf{e}$ is the polarization vector. Treating the kink in a harmonic trap (potential well) with angular frequency Ω and writing $\omega_0(\mathbf{k},s)$ for the angular frequency of the phonons results in the total Lagrangian

$$L = L_q + L_{z_0} + L_{\text{int}} + \text{const}, \quad (4)$$

$$L_q = \frac{\rho V}{2}\sum_{\mathbf{k},s}\left\{\dot q(\mathbf{k},s)\dot q^*(\mathbf{k},s) - \omega_0^2(\mathbf{k},s)q(\mathbf{k},s)q^*(\mathbf{k},s)\right\}, \quad (5)$$

$$L_{z_0} = \frac{M}{2}\left\{\dot z_0^2(t) - \Omega^2(z_0(t) - z_0^0)^2\right\}, \quad (6)$$

$$L_{\text{int}} = -i\rho V \sum_{j,\mathbf{k},s} k_z \dot z_0(t)\mathrm{e}^{-ik_z z_0(t)}\xi_0(k_z)\, F_j(\mathbf{k})\dot q^*(\mathbf{k},s)e_j^*(\mathbf{k},s). \quad (7)$$

In the equations above, ρ is the density of the crystal, $V = L^3$ its total volume, M is the kink mass [6], z_0 indicates the position of the kink, z_0^0 is its rest position and $F_j(\mathbf{k})$ is the Fourier transform of $f_j(\mathbf{r}_\perp : \kappa)$, being defined as

$$F_j(\mathbf{k}) \equiv \frac{1}{L^2}\int \mathrm{e}^{-i\mathbf{k}_\perp\cdot\mathbf{r}_\perp} f_j(\mathbf{r}_\perp : k_z)d^2 r_\perp, \quad (8)$$

where $\mathbf{k}_\perp = (k_x, k_y)$.

From the interaction term L_{int} one can determine the phonon–kink scattering amplitude per unit time $A(\mathbf{k}, s; \mathbf{k}', s')$. Due to phonon–kink scattering, phonons are no longer described by the Bose–Einstein distribution $N^0(\omega_0(\mathbf{k},s))$. In the presence of a small temperature gradient ∇T, the linear correction to the Bose–Einstein distribution $\delta N_{\mathbf{k}s}$ is given by

$$-\frac{\hbar\omega_0(\mathbf{k},s)}{k_B T^2} N^0(\omega_0(\mathbf{k},s))(1 + N^0(\omega_0(\mathbf{k},s))\,\nabla T \cdot \frac{\partial\omega_0(\mathbf{k},s)}{\partial\mathbf{k}} =$$

$$= \sum_{s'}\int \frac{d^3k'}{(2\pi)^3}\mathcal{P}(\mathbf{k},s;\mathbf{k}',s')[\delta\tilde N_{\mathbf{k}s} - \delta\tilde N_{\mathbf{k}'s'}] \quad (9)$$

with

$$\delta\tilde N_{\mathbf{k}s} = \frac{\delta N_{\mathbf{k}s}}{N^0(\omega_0(\mathbf{k},s))[1 + N^0(\omega_0(\mathbf{k},s))]}, \quad (10)$$

and

$$\mathcal{P}(\mathbf{k},s;\mathbf{k}',s') = N_{\text{ph}}L^2\,|\,A(\mathbf{k},s;\mathbf{k}',s')\,|^2 \times$$
$$\times K[\omega_0(\mathbf{k},s) - \omega_0(\mathbf{k}',s'); q_x, q_z]\times$$
$$\times N^0(\omega_0(\mathbf{k}',s'))[1 + N^0(\omega_0(\mathbf{k},s))] \quad (11)$$

with N_{ph} the number of phonons in the crystal and

$$K(\omega; q_x, q_z) = \frac{1}{L}\int dz dz' dt \exp[iq_z(z'-z) + i\omega t]\times$$
$$\times\langle\langle \exp[-iq_x\xi(z,0)]\exp[iq_x\xi(z',t)]\rangle\rangle. \quad (12)$$

With Eq. (9) a full kinematical treatment of the phonon–kink scattering is possible.

3. Heat flow

With the full kinematics of the phonon–kink scattering at our disposal we are able to study the effect of phonon–kink scattering on the heat flow through the crystal. The heat flux $\mathbf{Q}$ is given by

$$\mathbf{Q} = \sum_s \int \frac{d^3k}{(2\pi)^3}\hbar\omega_0(\mathbf{k},s)\frac{\partial\omega_0(\mathbf{k},s)}{\partial\mathbf{k}}\delta N_{\mathbf{k}s} \approx -\chi\nabla T, \quad (13)$$

where χ is the matrix of the thermal conductivity. For simplicity, we will assume here that this matrix only has two distinct diagonal elements and no off-diagonal elements

$$\chi = \begin{pmatrix} \chi_\perp & 0 & 0 \\ 0 & \chi_\perp & 0 \\ 0 & 0 & \chi_\parallel \end{pmatrix}. \quad (14)$$

This implies that there two distinct heat flows. One along the dislocation

$$Q_\parallel = -\chi_\parallel(\nabla T)_z, \quad (15)$$

and one perpendicular to,

$$Q_\perp = -\chi_\perp(\nabla T)_\perp, \quad (16)$$

with $(\nabla T)_\perp = ((\nabla T)_x, (\nabla T)_y, 0)$.

Combined Eqs. (9) and (13) allow for a full calculation [7] of $\chi_{\|}$ and $\chi_{\perp}$. This full calculation shows that there are four different temperature regimes for the thermal conductivity. These four intervals are

$$\begin{aligned} &\text{regime 1: } T \ll T_{\omega}, \\ &\text{regime 2: } T_{\omega} \ll T \ll T_{\Omega}, \\ &\text{regime 3: } T_{\Omega} \ll T \ll T^{*}, \\ &\text{regime 4: } T \gg T^{*}, \end{aligned} \tag{17}$$

Here

$$T_{\omega} = \frac{\hbar\omega_0(1/\ell)}{k_B}, \quad T_{\Omega} = \frac{\hbar\Omega}{k_B}, \quad T^{*} = \frac{2M\Omega^2\ell^2}{k_B}, \tag{18}$$

where ℓ is the typical size of the kink and $\omega_0(1/\ell)$ is the angular frequency for a phonon with a wavelength equal to the size of the kink. The three temperatures are ordered as follows:

$$T_{\omega} \ll T_{\Omega} \ll T^{*}. \tag{19}$$

In the calculations we also took into account that in real experiments, one does not measure the thermal conductivity in one particular direction, but rather an average over different direction as one has no perfect control of the orientation of the kinks. As the scattering in different directions is a consecutive process, the scattering rates for the different processes add. This means that the measured thermal conductivity $\tilde{\chi}$ is found from

$$\tilde{\chi}^{-1} = \beta\chi_{\perp}^{-1} + (1-\beta)\chi_{\|}^{-1}, \tag{20}$$

where $\beta \in [0,1]$.

Therefore, one ends up with the following scaling behavior for $\tilde{\chi}^{-1}$,

$$\tilde{\chi}^{-1} \sim n_{\text{ph}} \begin{cases} \beta + n_k \mathcal{C} T^{-4}, & \text{regime 1,} \\ \beta T^{-1} + n_k \left[\mathcal{C} T^{-5} + \mathcal{D} T^{-7} \right], & \text{regime 2,} \\ \beta T^{-1} + n_k \left[\mathcal{C}(1-\beta) T^{-5} + \mathcal{D}\beta T \right], & \text{regime 3,} \\ \beta T^{-1} + n_k \left[\beta T^{-3} + (1-\beta) T^{-5} \right] & \text{regime 4,} \end{cases} \tag{21}$$

where $n_{\text{ph}} = N_{\text{ph}} / L^2$ and $n_k = N_k / L$ are the phonon and kink densities, respectively. The script letters indicate other quantities than the ones expressed already in the equations above.

4. Comparison with experimental data and conclusion

We compare our qualitative theoretical results with experimental data in Ref. 1. In Fig. 1 of this reference one sees that for a sample of highly purified lead which has been plastically stretched at low temperatures, the thermal conductivity at low temperatures has a peculiar shape: up to certain temperature it increases with temperature, then starts decreasing and for even higher temperatures it starts increasing with temperature again. Annealing can make this effect less pronounced, but it seems not to be able to completely remove this feature. Assuming that β is neither 0 nor 1 and taking numerical results into account [7], one sees from Eq. (21) that for low temperatures $\tilde{\chi}$ scales as

$$\frac{T^4}{n_k \mathcal{C} + T^4}, \tag{22}$$

for higher temperatures as

$$\frac{T^5}{n_k \mathcal{C} + T^4}, \tag{23}$$

for even higher temperatures as

$$\frac{T^{-1}}{n_k \mathcal{C} + T^{-2}}, \tag{24}$$

and at the highest temperatures as

$$\frac{T^5}{n_k \tilde{\mathcal{C}} + T^4}. \tag{25}$$

This mimics the behavior shown in the experimental data. In the semi-highest temperature regime the thermal conductivity will decrease with temperature, while in the other regimes the thermal conductivity will increase with temperature.

When comparing curves *6* and *7* in Fig. 1 [1], one sees that curve *6* and *7* have similar behavior for higher temperatures. For lower temperatures though, curve *6* lies under curve *7*. As curve *6* shows the thermal conductivity for a sample which has been deformed, while curve *7* shows the thermal conductivity for a lead sample which has not been deformed at all, this is in full agreement with the theory. The power-law for the thermal conductivity for a sample with none or very little kinks has a lower power than that for a sample with many kinks. Therefore it makes sense that for low temperature, the thermal conductivity for a sample with many kinks is lower than that for a sample with very little kinks. For this observation, we can therefore conclude that samples which have not been plastically deformed at all show a much weaker version of this effect, proving that this effect is indeed caused by phonon–kink scattering. This also shows that only a small amount of kinks are needed to let this effect appear.

The experimental data for the normal state does not match with our theoretical calculations at all, since in the normal state the phonon contribution to the heat flux transport is much weaker than the electron contribution. Therefore the effect of phonon–kink scattering is not visible in that case.

We thus see that the results of our model qualitatively agree with the experimental data. For a quantitative comparison we refer to Ref. 7. The work of S.I.M. is in part supported by RFFI grant 12-02-01018.

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