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Disclinations as a source of thermal resistance in icosahedral i-AlPdMn quasicrystals

S E Krasavin

Joint Institute for Nuclear Research, Bogoliubov Laboratory of Theoretical Physics, 141980 Dubna, Moscow region, Russia

E-mail: krasavin@thsun1.jinr.ru

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Abstract
We propose a model to analyse the experimental data for thermal conductivity of single-grain i-AlPdMn quasicrystals. The interpretation is based on the picture in which disclination pairs of wedge type are the main source of phonon scattering at low temperatures. The scattering of phonons due to strain fields of these dipoles is considered. Our numerical calculations show that experimentally observed thermal conductivity in a wide temperature range can be well fitted by a combination of wedge disclination dipole scattering and quasi-umklapp scattering processes.

1. Introduction

Quasicrystals are solids with long-range quasiperiodic translation order and long-range orientational order [1–3]. Nevertheless, despite the high structural order of quasicrystals their transport properties resemble those of disordered materials [4]. In particular, it is established that icosahedral quasicrystals appear to have a glass-like thermal conductivity [5, 6]. Most of the early studies described the low-temperature thermal conductivity (below 1 K) of quasicrystals in the framework of the tunnelling states model (TLS) [5, 7]. If the appearance of the tunnelling states in amorphous materials can be explained by the presence of disorder, the physical nature of their existence in quasicrystals is not yet understood. Conceivably, tunnelling states can be induced by some particular type of disorder (e.g., phason disorder [8–10]). At present, in some works the low-temperature thermal conductivity of i-YMgZn and i-AlPdMn icosahedral quasicrystals has been considered without tunnelling states [11, 12]. The good fit for low and intermediate temperatures was reached with the assumption that the total relaxation rate is a combination of Casimir, stacking fault and quasi-umklapp scattering processes.

In this paper, we suggest an alternative mechanism of phonon scattering based on the concept of the rotational linear defects (namely disclinations) to explain the glass-like thermal conductivity of i-AlPdMn quasicrystals observed in [5]. These defects in real i-AlPdMn quasicrystals can appear as a result of icosahedra and icosidodecahedra close packing in three-dimensional space that leads to the frustration of local angular dependences between different neighbourhoods [13, 14]. As is known, direct observation of disclinations is problematic [15], as distinguished from dislocations, but their presence was confirmed in numerical simulations. In [16], it was shown numerically that the local topological frustration (i.e. local deviation from ideal icosahedral packing) associated with four- and six-fold disclinations is the reason for localized modes in quasicrystals. Disclinations have been discussed in the context of correlation between short-range icosahedral order in liquids and long-range icosahedral order in quasicrystals [17]. Recently, in [18], a local atomic structure of $Mg_{25}Y_{11}Zn_{64}$ icosahedral quasicrystals has been studied on the basis of synchrotron powder diffraction data and the real-space pair distribution function. Frank–Kasper polyhedra [19] with coordination numbers different from 12 were found. This type of polyhedron has been described in the literature as containing disclinations [15].

2. Model

To obtain the low-temperature quadratic law of thermal conductivity of i-AlPdMn observed in [5] we should suppose in our scheme that local strains over a quasilattice correspond to the wedge disclinations combined in dipole configurations. For particular dipole configurations (biaxial dipoles), as was shown in [20], the phonon mean free path is proportional to the inverse value of the wavevector in the long-wavelength limit that leads to T^2-dependence of thermal conductivity at low temperatures. In [21], the wedge disclination dipole (WDD) model has been successfully applied to fit the experimental thermal conductivity of dielectric glasses over a wide temperature range. The effect of other disclination defects (e.g. twist disclination dipoles, wedge disclination loop) on thermal transport has been analysed as well, and no glass-like thermal conductivity was found (see e.g. [22]).

In our picture we assume that biaxial WDDs are distributed in the XY-plane and their lines are oriented along the Z-axis. It should be mentioned that a chaotic distribution of disclination lines only modifies the absolute value of the phonon mean free path in calculations (see e.g. [23]). Supposing also that clusters contain disclinations, we take a distance between two disclinations ($2L$, the dipole separation) equal to the inter-cluster size. We consider WDDs where the axes of rotation are not shifted relative to disclination lines (biaxial WDDs). If the dipole arm is oriented along the x-axis, an effective perturbation energy due to the strain field caused by a single WDD is (see e.g., [21])

$$U(x, y) = \frac{\hbar q v_s \gamma \Omega (1 - 2\sigma)}{4\pi(1 - \sigma)} \ln \frac{(x + L)^2 + y^2}{(x - L)^2 + y^2}, \tag{1}$$

where q is the phonon wavevector, v_s is the sound velocity, γ is the Grüneisen constant, Ω is the axial vector (Frank vector) directed along the disclination line, and σ is the Poisson constant.

For the chosen geometry, in view of equation (1) the problem of scattering reduces to the two-dimensional case as for an edge dislocation [24]. Then, a mean free path arising due to the phonon scattering by static strain fields of WDDs within the generally accepted deformation potential approach is given by

$$l_D^{-1}(q) = 2A^2(\Omega L)^2 n_{dis} q \left(J_0^2(2qL) + J_1^2(2qL) - \frac{1}{2qL} J_0(2qL) J_1(2qL) \right), \tag{2}$$

where $A = \gamma(1 - 2\sigma)/(1 - \sigma)$, n_{dis} is the areal density of WDD, and $J_n(t)$ are Bessel functions. Notice also that to get equation (2) we considered the elastic scattering of phonons with wavevector q within the Born approximation. Taking $2L$ equal to 10 Å (the inter-Mackay icosahedron distance for i-AlPdMn [25–27]) and the specimen size from [5], we estimate the order of the WDD areal density value, $n_{\rm dis} \sim 10^{13}$ cm^{-2}. In equation (2) the Frank vector Ω is considered as a varying parameter.

The total mean free path is written as

$$l(\omega) = (l_{\rm D}^{-1}(\omega) + l_{\rm qu}^{-1}(\omega))^{-1} + l_{\rm min}. \quad (3)$$

The above formula has been widely used in literature [28, 29] to fit thermal conductivity with glass-like behaviour. $l_{\rm qu}$ is the mean free path due to quasi-umklapp processes (see [4]). To fit the experimentally observed thermal conductivity [5] for i-AlPdMn quasicrystals, we use a weaker temperature dependence for $l_{\rm qu}$ than that proposed in [4], where $l_{\rm qu} \propto \omega^2 T^4$. According to [30] it takes the form

$$l_{\rm qu}^{-1}(\omega) = B\frac{\omega^2}{v_{\rm s}}T^2, \quad (4)$$

where B is the fitting constant. The last term in equation (3) describes the least possible mean free path of propagating acoustic phonons. The experimental evidence for the $l_{\rm min}$ introduction in equation (3) follows from inelastic neutron scattering experiments in [25]. It was found that unbroadened acoustic modes can exist only when wavevectors $q \leqslant 0.35$ Å^{-1} that gives the value of the least mean free path $l_{\rm min} \sim 18$ Å.

To calculate the temperature dependence of thermal conductivity with the mean free path given by equation (3) we use the following kinetic formula written in the dimensionless form

$$\kappa = \frac{k_{\rm B}^4 T^3}{2\pi^2\hbar^3 v_{\rm s}^2}\int_0^{\Theta/T} x^4 {\rm e}^x({\rm e}^x - 1)^{-2} l(x)\,{\rm d}x, \quad (5)$$

where $k_{\rm B}$ and $\hbar$ are Boltzmann's and reduced Planck constants, Θ is the Debye temperature, and $x = \hbar\omega/k_{\rm B}T$.

3. Results

Figure 1 shows the experimental data for thermal conductivity over a wide temperature range of the i-AlPdMn sample from [5] together with theoretical curve. It is seen from the plot that there is a good agreement between the fitting curve and experimental data for T below approximately 10 K where $\kappa \sim T^2$. In our scheme, the main contribution to $\kappa(T)$ at lowest T is due to the phonon scattering by strain fields of a biaxial WDD. The best fit was found in calculations with Frank vector $\Omega \approx 5°$. One can obtain from equation (2), $l_{\rm D} \sim \omega^{-1}$ at $\lambda > 2L$, which leads to the observed $\kappa \sim T^2$ at low temperatures.

For $\lambda < 2L$, $l_{\rm D} \rightarrow$ constant, and the crossover to $\kappa \sim T^3$ takes place at $T^* \simeq \hbar v_{\rm s}/2Lk_{\rm B} =$ 25–30 K, if only the WDD source of scattering (2) is present instead of (3). The formula for T^* can be derived from the condition $\lambda \sim 2L$ using the dominant phonon approximation [21]. This crossover, however, is absent on the plot because of the dominating quasi-umklapp processes at these temperatures.

In the shallow maximum region for the temperature range 4 K $\leqslant T \leqslant$ 40 K a qualitative fit between calculated and experimental $\kappa(T)$ is seen in figure 1. This is the result of a combination of two scattering processes in the calculations: scattering due to biaxial WDD and quasi-umklapp scattering. We found in calculations that the value of $\kappa(T)$ in the region of the maximum (near 10 K) becomes higher if the stronger T-dependence of $l_{\rm qu}$ is used in equation (4) (e.g. $l_{\rm qu} \sim T^4$).

In our previous work [21] we investigated amorphous SiO_2 compounds where a plateau-like region is present as well. The good fit for $\kappa(T)$ was obtained by combining the biaxial WDD scatterer with the Rayleigh-type source of scattering. The mechanism proposed here leads to the strong decrease of $l(\omega)$ (plateau-like regime) at higher frequencies. As a result,

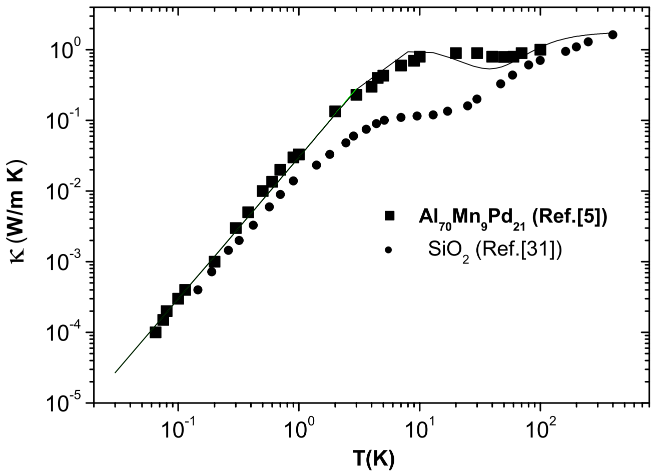

Figure 1. Quasilattice thermal conductivity versus temperature for the i-AlPdMn sample (dark squares) experimentally observed in [5]. The solid line is a fit according to equations (3) and (5) with fitting parameters $\Omega = 5°$, $B = 4 \times 10^{-18}$ s K^{-2}, $l_{min} = 10$ Å, using the following experimental values: $n_{dis} = 6 \times 10^{13}$ cm^{-2}, $\Theta = 380$ K, $v_s = 4 \times 10^5$ cm s^{-1}, $2L = 10$ Å. The data for amorphous SiO_2 (dark circles) are taken from [31].

(This figure is in colour only in the electronic version)

the plateau region of the quasilattice κ exists at higher temperatures than the constant κ of amorphous SiO_2 from [31]. In addition, the absolute value of the quasilattice κ in the T-independent region exceeds the corresponding value for SiO_2 with the same fixed parameters related to biaxial WDDs. This result is in agreement with that obtained in [5].

At temperatures above $T \approx 50$ K the experimental $\kappa(T)$ in figure 1 is slightly increased. The physical reason for this increase is, evidently, in opening of a new heat-carrying channel, e.g. the clustron hopping mechanism proposed in [26]. In our model this rise of κ is the result of formal l_{min} introduction (see details above in text). Interestingly enough, as was mentioned above, the average value of the dipole separation $2L$ has the same meaning as l_{min} (~10 Å). Thus, $2L$, or in other words, the local region of distortion between two adjoining icosahedral clusters, can serve as a parameter of phonon localization. An inter-cluster size as the possible origin of localization of the modes has been considered in [25].

In conclusion, a new view has been suggested to explain the experimentally observed thermal conductivity of icosahedral i-AlPdMn quasicrystals. Our mechanism implies that disclinations combined in dipole configurations are responsible for the phonon scattering at very low temperatures. At low and intermediate temperatures a good agreement between our model and experimental data was reached by a combination of disclination dipole and quasi-umklapp scattering mechanisms.

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