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The effect of surface roughness on the phonon mean free path in narrow wires

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Abstract. We discuss guided phonon propagation in extremely narrow wires with position modulated radius and free boundaries. The modulated radius represents a randomly rough surface associated with the fabrication of small wires. A coordinate transform technique is used to introduce the surface roughness into the vector differential equation for an elastically isotropic medium. By solving the secular equation numerically we have been able to determine the dependence of the phonon mean free path on wave vector, roughness amplitude and correlation length.

1. Introduction

Low temperature transport studies of free-standing wires have been of interest as a candidate for the observation of quasi-one-dimensional phonon transport. Jäckle [1] considered the thermal properties of such samples by extending the model for electron localization [2] to the case for phonons. It was predicted that the phonon localization length would be proportional to the cross-sectional area of the wire and to the inverse squared phonon frequency. Kelly [3] considered the low temperature properties of narrow, self-supporting wires. At temperatures for which the dominant phonon wavelength is of the order of the lateral dimensions of the wire, it was assumed that the wire behaved as a phonon wave guide and that the mean free path (MFP) was determined by length scales associated with the correlation length of surface roughness. With this model Kelly predicted that the MFP should be large compared to the lateral dimensions of the wire. As a consequence of the relatively long MFP it was expected that phonons would be very efficient at removing heat from a narrow wire.

Following this theoretical work, several attempts have been made to determine experimentally the phonon MFP in narrow wires [4, 5, 6]. In all cases the inferred MFP was much less than predicted. In an attempt to understand the discrepancy between the physically appealing wave guide model and the experimental data, we have performed a more complete analysis of the problem. Our results show how the model of Kelly [3] and the various experimental data may be reconciled.

In the elastic continuum limit, wire structures with free-boundaries have been shown to have many dispersion branches close to the zone-centre [7]. These branches arise from spatial quantization of the phonon spectrum and depend on the geometry of the wire. The fact that the free-surface determines the nature of the dispersion branches suggests that the surface irregularities will play an important role in phonon transport.

In this paper we determine the MFP of phonons in wires with random surface roughness. We adopt a method introduced to study the phonon spectra in similar structures [8] and we restrict our calculations to several of the lower dispersion branches.

2. Model

The displacement vector $\boldsymbol{u}$ for wave propagation in elastically isotropic media satisfies the wave equation:

$$\delta^2 \boldsymbol{u}/\delta t^2 = c_t^2 \nabla^2 \boldsymbol{u} + (c_l^2 - c_t^2) \operatorname{grad} \operatorname{div} \boldsymbol{u} \tag{1}$$

where c_t and c_l are the transverse and longitudinal velocities of sound. We have introduced surface roughness of a cylindrical wire by a modulation of the radius, $\mathbb{R} = R(1 + \chi f(z))$, where R is the wire radius and $\chi = A/R$ where A is the amplitude of roughness and $f(z)$ is the functional form of the surface profile. We solved equation (1) in cylindrical coordinates by looking for solutions of the form

$$\boldsymbol{u}(r, \theta, z) = \mathfrak{R}(r, z)\, \mathrm{e}^{\mathrm{i}qz}\, \mathrm{e}^{\mathrm{i}m\theta}\, \mathrm{e}^{\mathrm{i}\omega t} \tag{2}$$

where the radial part of the wave function, $\mathfrak{R}(r, z)$, incorporates the effect of the surface roughness. The coupling between the r and z components makes it impossible to solve equation (1) using a separation of variables technique.

To overcome this problem we have adopted the following coordinate transformation: $\imath = r(1 + \chi f(z))$, $z = z$ and $\theta = \theta$. We now can eliminate the derivatives with respect to z for each vector component of $\mathfrak{R}$ using the relation:

$$\frac{\delta \mathfrak{R}}{\delta z} = \frac{\delta \imath}{\delta z} \frac{\delta r}{\delta \imath} \frac{\delta \mathfrak{R}}{\delta r} = rZ \frac{\delta \mathfrak{R}}{\delta r}$$

where $Z = (\delta f(z)/\delta z)(1 + \chi f(z))^{-1}$ and so is a function of z only. The wave functions were then determined as power series by decoupling the longitudinal and the transverse components into $\boldsymbol{u} = \boldsymbol{u}_l + \boldsymbol{u}_t$ and using equation (3) to solve equation (1).

Restricting ourselves to the case for $m = 0$ and dropping the $\mathrm{e}^{\mathrm{i}\omega t}$ term, the two components of the wavefunction have the form:

$$\boldsymbol{u}_l \begin{pmatrix} r \\ \theta \\ z \end{pmatrix} = B \begin{bmatrix} \sum_\nu b_\nu \nu \beta (\beta r)^{\nu - 1} \\ 0 \\ \sum_\nu \left(\frac{\delta b_\nu}{\delta z} + \mathrm{i} q b_\nu \right) (\beta r)^\nu \end{bmatrix} \mathrm{e}^{\mathrm{i}qz}$$

$$\boldsymbol{u}_t \begin{pmatrix} r \\ \theta \\ z \end{pmatrix} = \left\{ A \begin{bmatrix} 0 \\ -\sum_\nu \alpha a_\nu \nu (\alpha r)^{\nu - 1} \\ 0 \end{bmatrix} + C \begin{bmatrix} \sum_\nu \left(\frac{\delta c_\nu}{\delta z} + \mathrm{i} q c_\nu \right) (\alpha r)^{\nu + 1} \\ \sum_\nu \left(\frac{\delta c_\nu}{\delta z} + \mathrm{i} q c_\upsilon \right) (\alpha r)^{\nu + 1} \\ -\sum_\nu c_\nu (\nu + 2) \alpha (\alpha r)^\nu \end{bmatrix} \right\} \mathrm{e}^{\mathrm{i}qz}$$

where a_ν, b_ν and c_ν are given by the recursion relations

$$a_\nu = \left(\frac{1}{\nu}\frac{1}{\alpha^2}(Z' + 2\mathrm{i}qZ - Z^2) + \frac{1}{\nu^2}\frac{Z^2}{\alpha^2}\right)a_{\nu-2} - \left(\frac{1}{\nu}\frac{1}{\alpha^4}Z^2(Z' + 2\mathrm{i}qZ + \alpha^2)\right)a_{\nu-4}$$

$$b_\nu = \left(\frac{1}{\nu}\frac{1}{\beta^2}(Z' + 2\mathrm{i}qZ - Z^2) + \frac{1}{\nu^2}\frac{Z^2}{\beta^2}\right)b_{\nu-2} - \left(\frac{1}{\nu}\frac{1}{\beta^4}Z^2(Z' + 2\mathrm{i}qZ + \beta^2)\right)b_{\nu-4}$$

$$c_\nu = \left(\frac{\nu-1}{\nu^2}\frac{1}{\alpha^2}(Z' + 2\mathrm{i}qZ - 3Z^2) - \frac{1}{\nu^2}\frac{Z^2}{\alpha^2}\right)c_{\nu-2} - \left(\frac{\nu-1}{\nu^2}\frac{Z^2}{\alpha^4}(Z' + 2\mathrm{i}qZ) + \frac{1}{\nu^2}\frac{Z^2}{\alpha^2}\right)c_{\nu-4}$$

where

$$\alpha^2 = \omega^2/c_\mathrm{t}^2 - q^2 \qquad \beta^2 = \omega^2/c_\mathrm{l}^2 - q^2$$

and the primes denote the differential with respect to z.

The solutions to the equations of motion have to satisfy the boundary condition that the surface of the wire be stress-free. This requires the normal components of the stress tensor T_{ij} to vanish on the surface: that is, $T_{\imath\imath} = T_{\imath\theta} = T_{\imath z} = 0$ at $\imath = \mathbb{R}$. The transformed stress tensor components $T_{\imath\jmath}$ are given by,

$$T_{\imath\jmath} = \sum \frac{\delta r}{\delta \imath}\frac{\delta j}{\delta \jmath} T_{rj}$$

and the relevant stress tensor components are given by

$$T_{rr} = \sum_\nu \left[B(c_\mathrm{l}^2 - 2c_\mathrm{t}^2)\left((8\nu^2\beta^2 - 2\nu\beta^2 - q^2)b_\nu + 2\mathrm{i}q\frac{\delta b_\nu}{\delta z} + \frac{\delta^2 b_\nu}{\delta z^2}\right)(\beta r)^{2\nu} + C\,2c_\mathrm{t}^2\alpha(4\nu^2 + 4\nu + 1)\left(\mathrm{i}qc_\nu + \frac{\delta c_\nu}{\delta z}\right)(\alpha r)^{2\nu+1}\right]\mathrm{e}^{\mathrm{i}qz}$$

$$T_{rz} = \sum_\nu \left[B\,2c_\mathrm{l}^2\beta(2\nu + 1)\left(\frac{\delta b_\nu}{\delta z} + \mathrm{i}qb_\nu\right)(\beta r)^{2\nu} - C\,2c_\mathrm{t}^2\left([(4\nu^2 - 4\nu)\alpha^2 + q^2]c_\nu - 2\mathrm{i}q\frac{\delta c_\nu}{\delta z} - \frac{\delta^2 c_\nu}{\delta z^2}\right)(\alpha r)^{2\nu+1}\right]\mathrm{e}^{\mathrm{i}qz}$$

$$T_{r\theta} = \sum_\nu \left[-A\,2c_\mathrm{t}^2\alpha^2(4\nu^2 - 4\nu)a_\nu(\alpha r)^{2\nu} + C\,2c_\mathrm{t}^2\alpha 2\nu\left(\mathrm{i}qc_\nu + \frac{\delta c_\nu}{\delta z}\right)(\alpha r)^{2\nu+1}\right]\mathrm{e}^{\mathrm{i}qz}$$

where A, B, C are constants. In the limit of small roughness amplitude we now expand the stress tensor components in powers of χ.

The phonon dispersion for different surface profile functions can be determined by equating the determinant of these stress tensor elements to zero. In this paper we are interested in random surface roughness. Thus we replace the specific surface profile function $\chi f(z)$ by a statistical ensemble of profile functions with the following properties. For brevity we drop the z dependence of $f(z)$ in the remainder of the paper. First, the average of the profile function $\langle \chi f \rangle$ is zero, second, the mean square of the profile function is given by $\langle(\chi f)^2\rangle = \chi^2$, third, the averages of all derivatives vanish, and fourth, the mean square of the nth derivative is given by

$$\langle(\mathrm{d}^n(\chi f)/\mathrm{d}z^n)^2\rangle = (2\chi/\xi^n)^2$$

where ξ is the correlation length of the roughness.

Using the properties mentioned above we can calculate the average coefficients $\langle a_\nu\rangle$, $\langle b_\nu\rangle$, and $\langle c_\nu\rangle$ and then use these to obtain the average stress tensor elements on the surface $\langle T^k_{ij}\rangle$, $j = r, \theta, z$; $k = a, b, c$. The coefficients are given by

$$\langle a_\nu\rangle = \sum_\nu (-\tfrac{1}{4})^\nu \frac{(\nu+1)}{\nu!^2}\bigg\{1 - \chi^2\bigg[(\nu^2 - 2\nu)\frac{q}{\alpha}\langle f^2\rangle + \bigg(\frac{6\nu^4 - 8\nu^3 - 8\nu^2 - 12\nu}{3}\alpha^2$$

$$+ \frac{3\nu^6 + 16\nu^5 + 4\nu^4 - 17\nu^3 - 104\nu^2 + 24\nu - 180}{6}q^2$$

$$+ (3\nu^4 + 8\nu^3 - 10\nu - 90)\frac{q^4}{\alpha^2}\bigg)\frac{\langle f'^2\rangle}{\alpha^4}$$

$$+ \bigg((3\nu^4 + 8\nu^3 - 10\nu - 90)(\nu^2 + 2\nu)\nu$$

$$+ \frac{3\nu^4 + 8\nu^3 - 10\nu - 90}{6}\frac{q^2}{\alpha^2}\bigg)\frac{\langle f''^2\rangle}{\alpha^4}\bigg]\bigg\}.$$

($\langle b_\nu\rangle$ has the same form as $\langle a_\nu\rangle$ but with α replaced by β) and

$$\langle c_\nu\rangle = \sum_\nu (-\tfrac{1}{4})^\nu \frac{(\nu+1)}{(\nu+1)!^2}\bigg\{1 + \chi^2\bigg[\bigg(\frac{6\nu^4 + 8\nu^3 - 8\nu^2 - 12\nu}{3}$$

$$- \frac{3\nu^4 + 8\nu^3 - 10\nu - 90}{6}\frac{q^2}{\alpha^2}\bigg)\frac{\langle f'^2\rangle}{\alpha^2} + \frac{3\nu^4 + 8\nu^3 - 10\nu - 90}{6}\frac{\langle f''^2\rangle}{\alpha^4}\bigg]\bigg\}.$$

Since the average of the surface profile function is zero, the lowest order of expansion of $\langle T^k_{ij}\rangle$ is second order in χ. The boundary conditions require $\langle T^k_{ij}\rangle$ to be zero on the surface, and so the phonon spectrum can be obtained by solving the secular equation $\det \mathbf{P} = 0$, where the elements of $\mathbf{P}$ are given by $P_{jk} = \langle T^k_{ij}\rangle$. This determinant can only be solved numerically. To obtain the phonon MFP we have to look for solutions of the form

$$\boldsymbol{u} = \mathfrak{R}(r, z; q, \omega)\,\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}qz}\,\mathrm{e}^{-z/l} = \mathfrak{R}(r, z; q, \omega)\,\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}(q_1 + \mathrm{i}q_2)z}$$

i.e. we search for solutions of ω versus $(q_1 + \mathrm{i}q_2)$. To avoid an elaborate search for zeros in the complex q-plane we adapted the following iteration procedure. $q_1(\omega)$ is given by the known dispersion curve of a perfectly cylindrical wire [7] and substituted into the secular equation, which subsequently has been solved for $q_2(\omega)$. Since we only considered the zeroth-order terms of q_1 we are not able to determine the dependency of the MFP on the roughness amplitude χ in this approximation. We now find the lowest order correction to $q_1(\omega)$ by solving the secular equation for $q_1(\omega)$ utilizing the calculated values of $q_2(\omega)$ and then using this corrected curve of $q_1(\omega)$ to solve for $q_2(\omega)$. After repeating this procedure several times the values of q_1 and q_2 converge towards the exact solution. We found that only few iterations were necessary to obtain a solution that is exact to one part in 10^3.

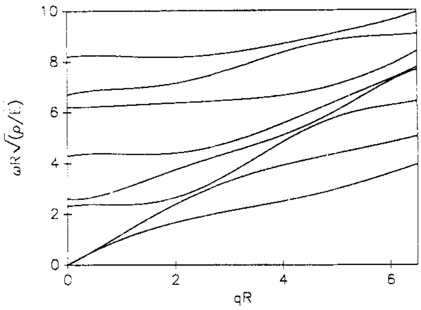

Figure 1. Phonon dispersion of a cylindrical wire without surface roughness. ρ and E are density and Young's modulus respectively. The velocity of sound ratio has been taken to be $c_l/c_t = 2$.

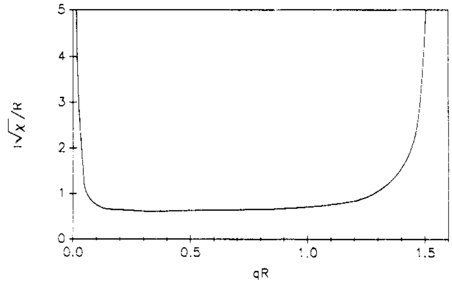

Figure 2. Dependence of the phonon MFP on the wave vector. The roughness correlation length has been taken to be $\xi = 5R$.

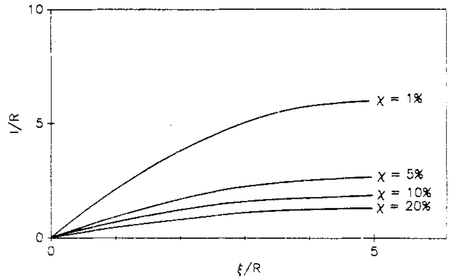

Figure 3. Dependence of the minimum value of the phonon MFP on the roughness correlation length ξ, shown for several roughness amplitudes.

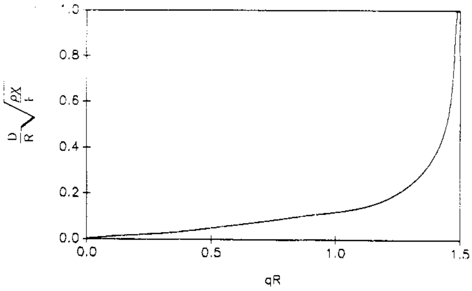

Figure 4. The scaled diffusion constant as a function of qR.

3. Results and discussion

Setting the roughness amplitude to zero, $\chi = 0$, we have calculated the phonon dispersion in a narrow wire, figure 1. This is in agreement with previously published data [7]. Using the usual definition of the MFP as the length over which the wave amplitude falls to $1/e$ of the initial amplitude, we have calculated the MFP for the lowest dispersion branch that does not emanate from the origin. We find the MFP to be proportional to $\chi^{-1/2}$ for χ between 0 and 0.3. In figure 2 we show the scaled MFP $l(\chi)^{1/2}/R$ as a function of qR. We find the MFP has a range of qR over which it is almost constant. Using different values of ξ, we have determined that for the wave vectors $0.5\xi^{-1} < q < 2\pi\xi^{-1}$ the MFP is almost constant. Outside this range the phonon wavelength becomes either greater than or less than the length scale associated with the surface roughness so, as expected, the phonons experience less interaction with the roughness and the MFP increases. For $q < 0.5\xi^{-1}$, we find the MFP to be proportional to q^{-2} while for $q > 2\pi\xi^{-1}$ the dependence follows a q^4 law. We note that in practice the long MFP for short wavelength phonons will be reduced by other scattering processes whose scattering cross section increase with wave vector, such as mass defect scattering.

The variation of the minimum value of the MFP as a function of the correlation length and amplitude of roughness is shown in figure 3. The MFP is found to vary as $\sim\xi^{1/2}$, and the dependence on the amplitude χ is $\sim\chi^{-1/2}$.

The ability of phonons to transport energy is described by the diffusion constant, $D(q) \simeq v_g(q)l(q)$. For small wave vectors, the phonon dispersion in branches that do not emanate from the origin can be expanded in terms of q: $\omega = \omega_n + \gamma q^2$, where ω_n is the frequency at the zone centre of the nth branch. From this expansion we can calculate the group velocity $v_g(\omega) = 2\gamma q$, and so estimate the diffusion constant for phonons in a particular branch. Figure 4 shows the scaled diffusion constant $(D/R)(\rho\chi/E)^{1/2}$ as a function of qR for the first branch. Close to the zone centre the diffusion constant is dominated by the low group velocity, thus the long MFP of the phonons is ineffective in transport. At larger values of qR, where the MFP increases, the MFP dominates the diffusion constant suggesting that higher wave vector phonons become more efficient at energy transport. As we mentioned previously, however, other phonon scattering mechanisms will act to reduce the MFP in this region.

We now compare our present results to previous work. For phonons with $q \ll 1/\xi$, $\xi = 10R$, and a mass fluctuation of 5%, corresponding to $\chi = 2.5\%$, Kelly [3] predicted the phonon MFP would be $\sim 4000R$. This is consistent with the present analysis in which we find a comparably large MFP for phonons of wavelengths $\gtrsim 2000R$. For wave lengths comparable to the roughness correlation length, phonon scattering by the surface roughness leads to a much shorter MFP. To compare our analysis with experiment we consider a wire of $R = 25$ nm having $\xi = 10$ nm and $\chi = 2\%$. At a lattice temperature of 1 K the dominant phonon wavelength is ~ 100 nm, $qR \sim 1.2$ and we find the MFP to be 300 nm; two orders of magnitude lower than anticipated previously and consistent with the available data.

4. Conclusion

We have calculated the wave vector dependence of the phonon MFP in narrow wires with randomly rough edges. Over a range of wave vectors, determined by the correlation length of the roughness, the MFP is almost constant and has a lower value than earlier calculations suggested. We have determined the variation of the phonon MFP as a function of the amplitude and correlation length of the roughness and have shown that scattering by surface asperities provides a mechanism for reducing the MFP in small wires.

Acknowledgment

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