ADP012717

TITLE: Giant Drop of the Lattice Thermal Conductivity Due to Confinement of Acoustic Phonons

This paper is part of the following report:

TITLE: Nanostructures: Physics and Technology International Symposium [6th] held in St. Petersburg, Russia on June 22-26, 1998 Proceedings

To order the complete compilation report, use: ADA406591

Ioffe Institute
6th Int. Symp. "Nanostructures: Physics and Technology"
St Petersburg, Russia, June 22–26, 1998.

Giant drop of the lattice thermal conductivity due to confinement of acoustic phonons

A. Balandin and Kang L. Wang
Device Research Laboratory, Electrical Engineering Department,
University of California – Los Angeles
Los Angeles, California 90095-1594 U.S.A.

Abstract. Lattice thermal conductivity of a quantum well was investigated taking into account dispersion of confined acoustic phonon modes. We show that strong modification of phonon group velocities due to spatial confinement leads to significant increase in the phonon relaxation rates and corresponding drop in the the lattice thermal conductivity (13% of the bulk value for 10 nm well). Our theoretical results are consistent with the recent experimental investigations of the thermal conductivity of a 155 nm wide Si_3N_4(150 nm)/Si(155 nm)/SiO_2(300 nm) quantum well conducted in our group.

1 Introduction

Thermal properties of semiconductor nanostructures and superlattices have recently attracted a lot of attention. To a large degree, this is due to a rebirth of the field of thermoelectric materials which was brought about by the emergence of large numbers of new artificially synthesized materials, including those structured on an atomic scale [1]. Recent reports that predicted strong enhancement of the figure of merit [2-3] ZT for semiconductor superlattices and quantum wells treated rigorously only electronic contribution, κ_e, to the thermal conductivity while ignoring the effects of spatial confinement on lattice contribution κ_l. In this report, we address the issue of how *spatial confinement of acoustic phonon modes directly modifies the lattice thermal conductivity* in a free-standing quantum well.

2 Theory

It is well known that the normal three-phonon scattering processes in which the total momentum is conserved cannot by themselves lead to a finite thermal resistance [4]. Only processes which do not conserve crystal momentum contribute to the lattice thermal resistance. Such processes are boundary scattering, impurity scattering, and three-phonon Umklapp scattering process in which the sum of phonon wave vectors is not conserved but changes by a reciprocal-lattice vector. Due to this reason, we will be primarily interested in examining the effects produced by phonon confinement on the above mentioned resistive processes. The electronic contribution, κ_e, is assumed to be small in undoped fully depleted semiconductor structures. In order to calculate κ_l, we use Callaway's expression for the thermal conductivity under the assumption that the resistive processes are dominant. Limiting our consideration to the above mentioned major contributions to the resistive processes, we can write the following relation for the relaxation rate

$$\frac{1}{\tau_C} = \frac{1}{\tau_U} + \frac{1}{\tau_B} + \frac{1}{\tau_I}, \tag{1}$$

where τ_U, τ_B, and τ_I are the relaxation times due to the Umklapp processes (all allowed channels), boundary scattering, and impurity scattering, respectively. We find the relaxation rate of the U-process for a thermal mode from the first-order perturbation theory. The derivation is somewhat complex and is reported elsewhere. The impurity scattering mechanism, which is affected by spatial confinement the most through the group velocity, is so-called isotope scattering arising from the presence of atoms with different mass. The relaxation time for this type of impurity scattering can be written as

$$\frac{1}{\tau_I} = \frac{V_0\omega^4}{4\pi v_g^3}\sum_i f_i[1-(M_i/M)]^2, \qquad (2)$$

where V_0 is the volume per atom, M_i is the mass of an atom, f_i is the fractional content of atoms with mass M_i which is different from M. The relaxation time for the boundary scattering can be evaluated from the semi-empirical relation $1/\tau_B = v_g/W$, where W is some characteristic thickness of a bulk semiconductor or the width of a quantum well. In order to evaluate relaxation times, we should use the actual dispersion relations and group velocities $v_g \equiv v_g(\omega(q))$ for phonons in a quantum well, where q is the wave vector. The modification of wave vector selection and frequency conservation rules due to the spatial confinement should also be taken into account.

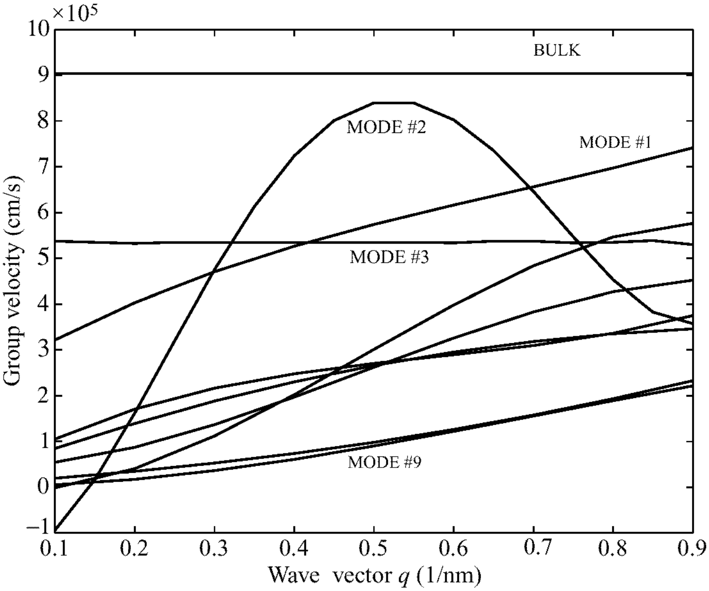

Fig 1. Group velocity as a function of the in-plane wave vector for the dilatational modes in a 10 nm wide Si quantum well. The dashed lines show the group velocity for bulk longitudinal acoustic phonon modes.

We find confined phonon modes from the elastic continuum approximation [5]. The normal components of the stress tensor on the free-standing quantum well must vanish. These boundary conditions, substituted instead of *periodic boundary conditions* of the bulk material, bring about a significant change to the phonon dispersion and group velocities. One should note here that a significant modification of phonon modes can be attained not only in a free-standing quantum well but also in a quantum well embedded in rigid material (Si_3N_4 for example) or in a heterostructure with relatively large difference of lattice constants. There are three different types of confined acoustic modes characterized by their distinctive symmetries: shear (S) waves, dilatational (D) waves, and flexural (F) waves, as compared to two types of the bulk modes: transverse (T) and longitudinal (L). The group velocities for the S and D modes in a 100 Å wide Si quantum well are shown on Fig. 1. It is easy to see that there are more dispersion and velocity branches for each polarization type as compared to the bulk, and group velocities of all branches decrease. The higher the mode number the smaller the group velocity. Since $\tau_I \propto v_G^3$, even a small decrease in the group velocity leads to a giant increase in phonon relaxation rates. The change of polarization types and the $\omega \equiv \omega(q)$ dependence brings also modifications of the energy and momentum conservation laws. It is known that for isotropic semiconductor only two general types of processes are allowed: $T + T \leftrightarrow L$, or $L + T \leftrightarrow L$. This restriction follows from the requirement that (i) all three interacting modes cannot belong to the same polarization branch, and (ii) the resultant mode should be above two initial (interacting) modes. It turns out that for confined acoustic phonons, the D mode is almost always above the S mode corresponding to the same branch n, and the processes $D_n + S_n \leftrightarrow D_n$ and $S_n + S_n \leftrightarrow D_n$ are *allowed* and can be treated by analogy with the bulk processes.

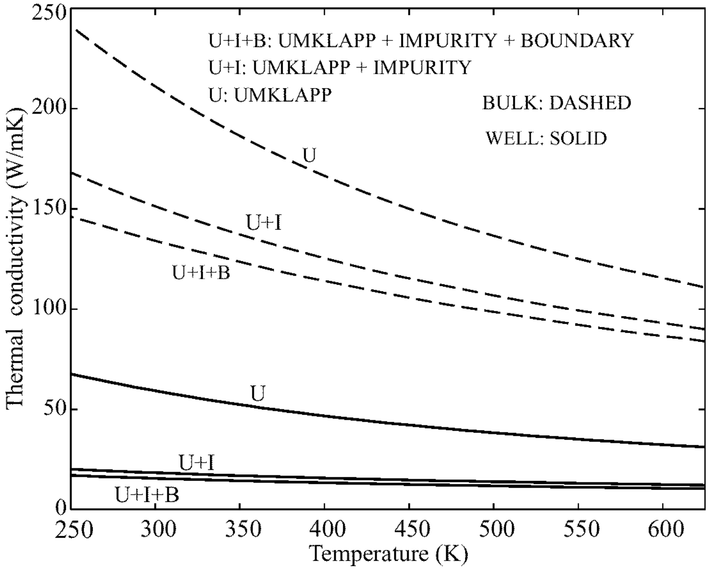

Fig 2. Lattice thermal conductivity as a function of temperature for bulk material (dashed) and the quantum well (solid).

3 Results and Discussion

We evaluate phonon scattering rates for a bulk Si 10 μm thick slab and Si 10 nm and 155 nm wide quantum wells. The material parameters used in simulation were the following: $a = 5.45$ Å, $\rho = 2.42 \times 10^3$ kg/m^3, $M = 46.6 \times 10^{-27}$ kg, $n_a \approx 7.3$, $\gamma = 0.56$, and $\theta = 625$ K. Numerical results show that the overall scattering rate increases in a quantum well. This increase is a direct result of the modification of phonon dispersion due to spatial confinement of the phonon modes. The later leads to the reduction of the group velocity which strongly increases the impurity and Umklapp scattering. In Fig. 2 we show the lattice thermal conductivity as a function of the temperature for the quantum well and the bulk material. In order to illustrate the contribution of different scattering mechanisms to the thermal resistivity, the conductivities limited only by the Umklapp scattering and by the Umklapp and impurity scattering are also shown. The overall thermal conductivity of a quantum well at 300 K is about 13% of the bulk Si. The calculated value and temperature dependence of the thermal conductivity are consistent with the results of the experimental investigation recently reported by some of us [6]. The measurements were conducted with a suspended microstructure which served as a thermal bridge. These measurements have shown that the lateral thermal conductivity of a Si_3N_4 (150 nm) / monocrystalline Si(155 nm) / SiO_2 (300 nm) structure was about 1.5% of the conductivity of the bulk Si and was almost a constant in the temperature range from $T = 293$ K to $T = 413$ K. Although our model assumed a free-standing quantum well, the results can be extended to quantum wells with rigid boundaries by appropriate modification of the boundary conditions. Our model applied to a 155 nm wide Si well gives $k_l = 66.7$ W/m K. For comparison, experimentally measured thermal conductivity of bulk Si is 148 W/m K. This is a significant drop although much less then that observed in the experiment. The temperature dependence of the calculated k_l is very close to the measured one. The discrepancy in the absolute value maybe due to (i) underestimated in our model boundary scattering, (ii) presence of other defect scattering processes [7], or (iii) crystal anisotropy, strain effects and related phonon focusing.

This work was supported by the DoD MURI-ONR program on Thermoelectrics and DoD MURI-ARO program on Low Power Electronics.

References

[1] For a recent review see G. Mahan, B. Sales, J. Sharp, *Physics Today*, **50** No.3 42 (1997).
[2] L.D. Hicks, M.S. Dresselhaus, *Phys. Rev. B*, **47** 12727 (1993).
[3] L.D. Hicks, T.C. Harman, M.S. Dresselhaus, *Appl. Phys. Lett.*, **63** 3230 (1993).
[4] P.G. Klemens, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1958), Vol. 7, p. 1;
Y.-J. Han, P.G. Klemens, *Phys. Rev. B*, **48** 6033 (1993).
[5] A. Svizhenko, A. Balandin, S. Bandyopadhyay, M.A. Stroscio, *Phys. Rev. B*, Feb. 15, (1998).
[6] X.Y. Zheng, S.Z. Li, M.Chen, K.L. Wang, in Proceed. of IMEC'96, Atlanta, Georgia, Nov. 17-22, 1996.
[7] A. Balandin, K.L. Wang, in proceed. of *American Physical Society*, Los Angeles, CA, USA, March, 1998.