UDC 538.9

PHONON THERMAL CONDUCTIVITY OF Si/Ge MODULATED NANOWIRES

A. Cocemasov[1], M.Sc., D. Nika[1], PhD, A. A. Balandin[2], PhD

[1] Department of Theoretical Physics, E. Pokatilov Laboratory of Physics and Engineering of Nanomaterials, Moldova State University
Republic of Moldova, Chisinau
[2]Nano-Device Laboratory, Department of Electrical Engineering,
Bourns College of Engineering, University of California–Riverside,
Riverside, California, USA
kocemasov@live.ru

We have shown theoretically that a combination of cross-section modulation and acoustic mismatch in the core/shell Si/Ge nanowires can lead to a three-orders-of-magnitude reduction of the thermal conductivity as compared to bulk silicon. Our results suggest that the acoustically mismatched cross-section modulated nanowires are promising candidates for thermoelectric applications.

Keywords: modulated nanowires, phonon thermal conductivity, phonon engineering.

Spatial confinement of acoustic phonons in semiconductor thin films and nanowires (NWs) can change their properties in comparison with the corresponding bulk materials [1—4]. Here we report the phonon engineering approach for thermal flux (TF) inhibition that does not rely on additional roughening of the interfaces. The latter allows one to reduce degradation of the electron mobility [5].

The schematic view of Si/Ge core-shell modulated nanowire (MNW) is shown in Fig. 1. It consist of two periodically repeated Si segments with dimensions $d_x^1 \times d_y^1 \times l_z^1$ and $d_x^2 \times d_y^2 \times l_z^2$ covered by Ge shell with the thickness d_{Ge}.

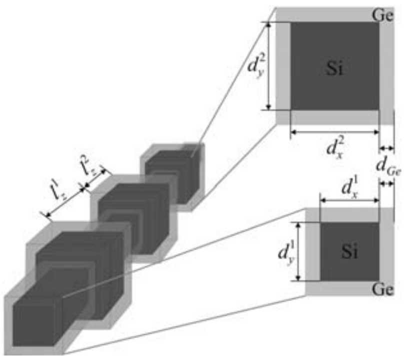

Fig. 1. Schematic view of Si/Ge core/shell modulated nanowire.

The calculations of the phonon thermal flux Θ per unit temperature gradient in the MNWs were performed using the expressions derived in Refs. [6—7] from the Boltzmann transport equation:

$$\Theta = \frac{1}{2\pi k_B T^2} \sum_{s=1,...,3N} \int_0^{\omega_{s,\max}} [\hbar\omega]^2 \upsilon_{z,s}(\omega) \tau_{tot,s}(\omega) \exp(\hbar\omega/[k_B T]) \left[\exp(\hbar\omega/[k_B T]) - 1\right]^{-2} d\omega \quad (1)$$

Here $\upsilon_{z,s} = d\omega_s / dq_z$ is the phonon group velocity along the MNW axis, k_B is the Boltzmann's constant, $\hbar$ is the Planck's constant, T is the absolute temperature, s enumerates the phonon branches and $\tau_{tot,s}(\omega)$ is the total phonon relaxation time for phonon mode (s,ω).

The dependence of the ratio of TF at room temperature for MNWs and Si NWs on d_{Ge} is presented in Fig. 2 for N_z = 4, 6, 8, 12. Two points for N_z = 20 and 28 at d_{Ge} = 4 ML are also shown. All curves demonstrate a maximum between d_{Ge} = 3 ML and d_{Ge} = 6 ML. The increase in N_z leads to a shift of the maximum to lower values of d_{Ge}. The difference between TF in MNWs and NWs becomes larger with growing N_z and it reaches the maximum values of 10—11 at $N_z \approx 28 - 32$ ML. For $N_z > 32$ ML, TF ratio starts to decrease due to redistribution of the phonon energy spectra and heat conduction through Ge shell.

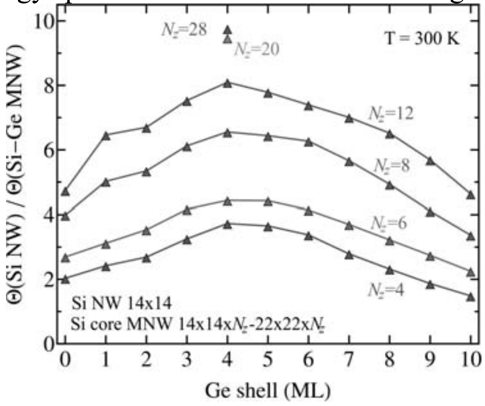

Fig. 2. Ratio of thermal fluxes in Si NW and Si/Ge MNWs as a function of N_z

The described approach for inhibition of the phonon thermal transport that does not rely on additional surface roughening can be achieved with relatively smooth interfaces, thus extending the possibilities of the phonon spectrum engineering. At room temperature, the 3—6 ML – thick Ge shell suppresses TF in Si/Ge MNW by an order of magnitude in comparison with Si NW and by a factor of two in comparison with Si MNW without cladding. As a result, phonon thermal conductivity of Si/Ge MNWs is almost three orders of magnitude lower than that of bulk Si.

Authors acknowledge the financial support from Moldova State (projects 11.817.05.10F, 14.819.16.02F, 14.820.18.02.012 STCU.A/5937) and STCU foundation (Project #5937).

REFERENCES

1. E. P. Pokatilov, D. L. Nika, A. A. Balandin. A phonon depletion effect in ultrathin heterostructures with acoustically mismatched layers // Appl. Phys. Lett. – 2004. – Vol. 85. – P. 825.
2. E. P. Pokatilov, D. L. Nika, A. A. Balandin. Confined electron-confined scattering rates in wurtzite AlN/GaN/AlN heterostructures // J. Appl. Phys. – 2004. – Vol. 95. – P. 5626.
3. E. P. Pokatilov, D. L. Nika, A. A. Balandin. Acoustic-phonon propagation in rectangular semiconductor nanowires with elastically dissimilar barriers // Phys. Rev. B. – 2005. – Vol. 72. – P. 113311.
4. A. A. Balandin, D. L. Nika. Phononics in low-dimensional materials // Materials Today.– 2012.– Vol. 15.– P. 266.
5. X. Zianni. Diameter-modulated nanowires as candidates for high thermoelectric energy conversion efficiency // Appl. Phys. Lett. – 2010. – Vol. 97. – P. 233106.
6. D. L. Nika, A. I. Cocemasov, C. I. Isacova, A. A. Balandin, V. M. Fomin, O. G. Schmidt. Suppression of phonon heat conduction in cross-section-modulated nanowires // Phys. Rev. B. – 2012. – Vol. 85. – P. 205439.
7. D. L. Nika, E. P. Pokatilov, A. A. Balandin, V. M. Fomin, A. Rastelli, O. G. Schmidt. Reduction of lattice thermal conductivity in one-dimensional quantum-dot superlattices due to phonon filtering // Phys. Rev. B. – 2011. – Vol. 84. – P. 165415.

А. Кочемасов, Д. Ника, А. Баландин

Фононная теплопроводность в Si/Ge модулированных нанонитях.

Теоретически показано, что комбинация модуляции поперечного сечения и акустического несоответствия в Si-нанонитях, покрытых оболочкой Ge, может привести к падению теплопроводности на три порядка по сравнению с объемным кремнием. Полученные результаты показывают, что нанонити с модуляцией поперечного сечения и акустическим несоответствием перспективны для применения в термоэлектричестве.

Ключевые слова: *модулированные нанонити, фононная теплопроводность, фононная инженерия.*