PHONON TRANSPORT IN AMORPHOUS SILICON NANOWIRES

Dmitrii CRISMARI, Denis NIKA

Among the perspective research directions in modern physics, the investigation of amorphous nanostructures plays an important role [1, 2]. The effect of the drop in lattice thermal conductivity in these compounds can be used in thermoelectric applications [3, 4].

Amorphous state of matter is characterized by an atomic structure with the short-range order, as characteristic for crystal structures the long-range order is absent [5, 6]. In this study, we theoretically investigated the phonon transport in amorphous silicon nanowires. Phonon energy dispersions are calculated at various degrees of amorphization in nanowires with dimensions of a few monolayers. Amorphization of nanowire crystal lattices was achieved by varying the parameters of interatomic interactions within the Valence Force Field (VFF) model of crystal lattice vibrations [7, 8]. In the calculation of the energy spectrum of amorphous nanowires, we took into account the following mechanisms of interatomic interactions: the two-particle "stretching", the three-particle "bending", "stretching-stretching", "stretching-bending" and the four-particle "bending-bending". In Figure 1 we present variation of phonon properties in amorphous silicon nanowires with 8x8 monolayers (ML) square cross-section for different percent of interatomic force constant variation.

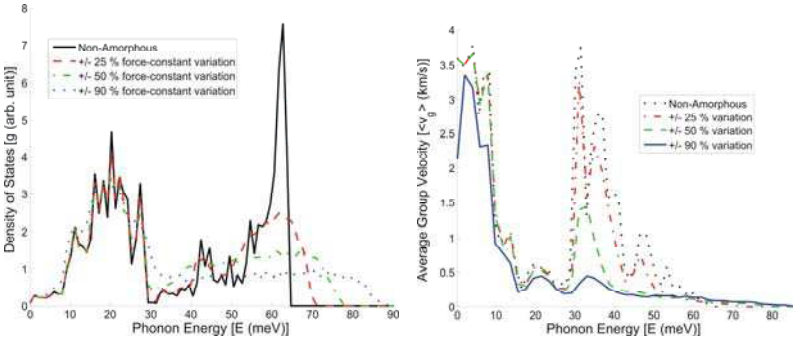

Fig. 1. (on the left) Phonon densities of states in crystalline and amorphous silicon nanowires with different degree of amorphization. (On the right) Average group velocities of phonons in crystalline and amorphous Si nanowire with different degree of amorphization

Change in degree of amorphization of nanowire crystal lattice leads to the substantial change both in phonon density and group velocity for modes with $\omega > 30$ meV. Our calculations show that thermal conductivity of the silicon nanowire with 8x8 ML square cross-section, calculated at room temperature, decreases from ~ 4.5 W/m·K for the crystalline silicon nanowire to ~ 2.8 W/m·K for the amorphous nanowire with amorphization 90 %. The later is explained by the modification of phonon density of states and phonon velocities.

References:

1. ZORN, R. Boson peak in confined disordered systems. In: *Phys. Rev. B*. 2010, vol. 81, p. 054208-1-054208-10.
2. SCHIRMACHER, W., DIEZEMANN, G., and GANTER, C. Harmonic Vibrational Excitations in Disordered Solids and the "Boson Peak". In: *Phys. Rev. Lett*. 1998, vol. 81, p. 136-139.
3. WADA, H. and KAMIJOH, T. Thermal Conductivity of Amorphous Silicon. In: *Jpn. J. Appl. Phys*. 1996, vol. 35, p. L648-L650.
4. LEE, Y.H., BISWAS, R., SOUKOULIS, C.M., WANG, C.Z., CHAN, C.T., and HO, K.M. Molecular-dynamics simulation of thermal conductivity in amorphous silicon. In: *Phys. Rev. B*. 1991, vol. 43, p. 6573-6580.
5. ФЕЛЬЦ, А. *Аморфные и стеклообразные неорганические твёрдые тела*. Москва: Мир, 1986. ISBN 978-5-458-41768-6.
6. БРОДСКИ, М., КАРЛСОН, Д., КОННЕЛ, Дж. *Аморфные полупроводники*. Москва: Мир, 1982. ISBN 978-3-540-16008-3.
7. CAMACHO, D. and NIQUET, Y.M. Application of Keating's valence force field model to non-ideal wurtzite materials. In: *Physica E*. 2010, vol. 42, p. 1361-1364.
8. TUBINO, R., PISERI, L., and ZERBI, G. Lattice Dynamics and Spectroscopic Properties by a Valence Force Potential of Diamondlike Crystals: C, Si, Ge, and Sn. In: *J. Chem. Phys*. 1972, vol. 56, p. 1022-1039.

Acknowledgements

Authors acknowledge the financial support from the Moldova State university projects no. 11.817.05.10F and 12.819.05.18F.