FP7-PEOPLE-2013-IEF
Final Report - HeatProNano (628197)

1. FINAL PUBLISHABLE SUMMARY REPORT

The ability to control and exploit heat propagation and thermal conductivity in low-dimensional semiconductor nanostructures constitutes one of the main challenges for the continued miniaturisation of electronic components. It is essential in the development of many technological devices such as thermoelectrics, nano- and optoelectronics, fuel cells, solar cells, thermal barrier coatings, and low thermal conductivity materials. As a consequence, the control of thermal energy quanta on the nanoscale is considered a crucial prerequisite for a variety of scientific and technological advances in the emerging field of nanoscale energy management.

The general aim of the Marie Curie IEF project HeatProNano (Heat Propagation and Thermal Conductivity in Nanomaterials for Nanoscale Energy Management) was to investigate, model, and exploit the heat propagation in different materials at the nanoscale. One class of nanostructures which is attracting increasing attention in this regard are free standing membranes. Prominent examples are single-atomic layers such as graphene and ultra-thin Si membranes which are applied to fabricate highly sensitive force-, mass-, and pressure sensors, low-loss macromolecule separators, microphones and micro-speakers, bolometres, and optomechanic cavities to name but a few. Moreover, the lack of interaction with a substrate and the capability of nanometre precise fabrication control promotes these types of nanostructures to ideal model systems for the experimental and theoretical study of the fundamental physical mechanisms of heat propagation and thermal conductivity at the nanoscale.

The work in the project HeatProNano was focused on ultra-thin membranes of silicon, germanium, and metal-oxides with varying thicknesses from a few nanometres to hundreds of nanometres. The fabrication and supply of the different samples was realized in collaborations with different groups and institutes in the European research community in the field of nanofabrication. Structural modifications of the membranes were introduced through regular (ordered) and irregular (disordered) hole patterning. The so fabricated 2D phononic crystals were investigated regarding their modification of the acoustic phonon dispersion relation, coherent acoustic phonon dynamics, and thermal conductivity. In addition, the project HeatProNano has investigated the transition between different heat transport regimes and has developed techniques to control and tailor the thermal conductivity at the nanoscale. The different scattering mechanisms which dominate the heat transfer efficiency of the thermal phonons were assessed in order to understand their relative contributions. Moreover, HeatProNano has analysed the regime of local non-equilibrium states in nanoscale structures with dimensions well below the mean free path of thermal phonons.

Several state-of-the-art optical spectroscopy techniques were designed, implemented, and applied during the funding period of the project in order to study the thermal conductivity, thermal diffusivity, coherent acoustic phonon dynamics, and acoustic phonon dispersion relations in these kind of materials. These include 2-laser Raman thermometry, frequency domain thermoreflectance, femtosecond pump & probe reflectivity spectroscopy based on an asynchronous optical sampling technique, Brillouin light scattering, and scanning thermal microscopy. The combination of these techniques has resulted in a multitude of new information about the phononic properties and nanoscale thermal processes in these materials.

Some of the scientific highlights achieved during the duration of the project include:

- Demonstration of the tuning of coherent and non-coherent phonon regimes by short range disorder in 2D phononic crystals:

  It was shown that short range disorder results in a pronounced modification of the phonon properties (dispersion, coherence) in the hypersonic range while leaving the thermal properties unaffected. Based on the experimental data and theoretical modelling, a general criteria for phonon coherence as function of roughness and disorder was derived and used to explain why the room temperature thermal conductivity in lithographically patterned structures is typical not affected by phonon coherence. These findings have important remnifications for novel phononic crystal based applications in RF communication technologies and optomechanics which depend on the ability to modify the phonon dispersion relation and thus the group velocity of acoustic phonons. Using controlled levels of disorder these results might pave the way towards a new class of disordered phononics in analogy to the already actively applied field of disordered photonics.

- Tuning thermal transport in ultra-thin membranes by surface nanoscale engineering:

  Silicon provides an ideal platform to study the relations between structure and heat transport since its thermal conductivity can be tuned over more than 2 orders of magnitude by nanostructuring and size reduction. Using a combination of atomistic modeling and experiments, the origin of the thermal conductivity reduction in ultrathin suspended silicon membranes was investigated down to a thickness of 4 nm. It was shown that heat transport is mostly controlled by surface scattering where rough layers the native oxide at the surfaces limit the mean free path of thermal phonons below 100 nm. In addition, it was shown that the removal of the native oxide layers by chemical processing allows to increase the thermal conductivity by more than 1 order of magnitude for ultra-thin membranes. The results have important implications for the materials design of future phononic applications since they define the length scale at which nanostructuring affects thermal phonons most effectively.

- Modification of phonon dispersion relation and thermal conductivity in ultra-thin Si membrane based 2D phononic crystals.

  The dispersion relation and thermal properties of 2D phononic crystals made of Si membranes with different characteristic dimensions (thickness, hole spacing and hole diameter) was investigated by inelastic light scattering techniques (Brillouin light scattering and 2 laser Raman thermometry). The measured phononic crystals showed significant changes in the acoustic phonon propagation due to Bragg scattering with respect to the Si membrane. The symmetry, localization and polarization of the acoustic modes in the phononic crystals could be successfully modelled using finite element method (FEM) simulations. Moreover, it was shown that thermal properties of the phononic crystals can be tuned in a simple and efficient manner by changing the neck size between the holes of the phononic crystal lattice. The thermal conductivity in the phononic crystals can be reduced at best by a factor of 40 with respect to the value of bulk Si at room temperature and thereby approaches the amorphous limit of Si with thermal conductivity of $1.7 Wm^{-1}K^{-1}$ while maintaining a feature size which is significantly larger than the electron mean free path in highly doped Si. These results are encouraging for the application of nano-scale engineered Si based structures as thermoelectric devices operating at high temperatures.