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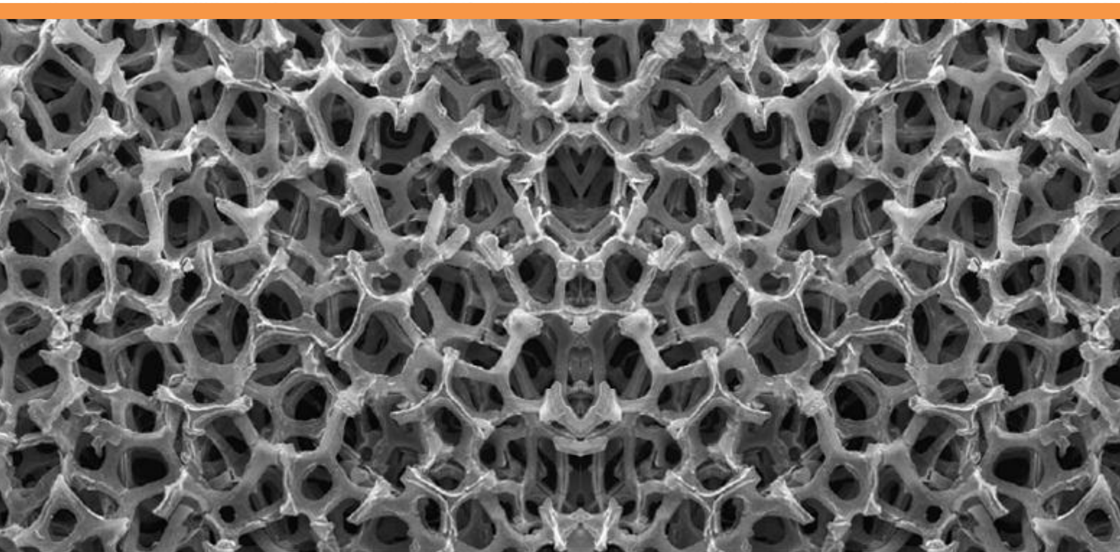

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Effects of Phonon Confinement in Ultra-Thin Silicon Membranes

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Understanding the behaviour of phonons in structures with reduced dimensions and, consequently, the effects on thermal properties of nanostructures is becoming more and more important due to miniaturization of devices. In the literature there is an increasing collection of theoretical papers on various aspects of nanophononics but experimental verification of the models has proven to be challenging. Ultra-thin membranes provide one way to probe the effects of acoustic phonon confinement on thermal properties and since the early experiments [1, 2] there has been increasing activity in the field. In this presentation we describe the recent advances in fabrication of ultra-thin, sub-10 nm thick, free-standing silicon membranes [3], development of new characterization techniques for heat propagation based on Raman spectroscopy [4], and the consequences of acoustic phonon confinement on phonon dispersion and phonon lifetimes [5, 6].

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Ultrafast Phononics in Membranes and Nanostructures

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The dynamics of acoustic phonons can be traced with high sensitivity in femtosecond pump-probe experiments. We investigate coherent acoustic phonons in different single-layer and double membrane systems as well as the acoustic dynamics of single nanostructures. We apply the method of high-speed asynchronous optical sampling which is based on two asynchronously locked femtosecond laser oscillators with approximately 1 GHz repetition rate. This method allows us to detect reflectivity changes below 10^{-7} within a few minutes of measurement times over 1 ns time delay with 50 fs resolution [1,2]. A model system for confined acoustic phonons are free-standing Si membranes [3-5]. A superposition of coherent confined longitudinal acoustic modes of odd order is observed after impulsive optical excitation [4]. The lifetime of these modes exceeds 5 ns at room temperature. This allows us to resonantly drive these modes by adjusting the repetition rate of the pump laser (1 GHz) to a sub-harmonic of the fundamental acoustic mode (19 GHz). By tuning the repetition rate we can map out the resonance excitation profile of the confined modes and accurately determine the Q factor [5]. This method is promising for the investigation of coherent excitation and selective amplification of acoustic modes of single nanostructures. In a double layer membrane system of aluminum and silicon we demonstrate the generation of an acoustic frequency comb combined of 24 modes of even and odd order spanning a frequency range from 12 GHz to 300 GHz [6]. The lifetime of each mode can be accurately determined giving a quantitative measure of frequency dependent damping times over the full frequency range in a single measurement.

The dynamics of single nanostructures is investigated for a silicon nitride doubly clamed beam [7]. Beams with two different clamping conditions are investigated. By calculating the strain integral on the surface of the resonators, we are able to reproduce the effect of the detection mechanism and identify all the measured modes. We show that our spectroscopy technique combined with our modelling tools allow the investigation of several different modes in the super high frequency range (3-30 GHz) and above, bringing more information about the vibration modes of nanomechanical resonators.

References

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Terahertz Acoustoelectric Devices using Semiconductor Nanostructures

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The development of the field of nanophononics as a tool for probing nanostructures, controlling thermal process in nanodevices, generation and manipulation of terahertz (THz) electromagnetic signals and as a potential new concept for quantum technology would be advanced through the development of a range of acoustoelectric devices for THz frequencies. Such devices would interface between the phononic and electronic domains, and are the phononic analogue of the optoelectronic devices, e.g. lasers and photodiodes, in nanophotonics.

Acoustoelectric effects are widely exploited in technology nowadays. Applications include: transducers for audio and ultrasonic frequencies and radiofrequency components such as surface acoustic wave (SAW) delay lines and band pass filters for used in communications devices. However, the maximum working frequency of current technologies is in the gigahertz (GHz) range. Generation and detection of coherent phonons in the THz and sub-THz frequency ranges presently requires the use of complex and costly femtosecond laser-based setups and is largely restricted to research laboratories possessing the necessary equipment and skills.

We have been investigating electronic devices based on semiconductor nanostructures for the generation and detection of Sub-THz coherent phonons. These include saser (or sound laser) devices [1] and detectors based on the piezojunction and high-frequency acoustoelectric effects in electron tunnelling devices [2, 3] and Schottky junctions [3]. In this talk I will explain the principles of operation of a few of these devices and show an example of how they can be integrated in a single-chip nanophononic device for the amplified detection of sub-THz coherent phonons.

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The high throughput approach in the search for novel materials

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The search for novel materials with improved tailored properties can be substantially accelerated with the help of ab initio high throughput computation. This is especially interesting in high priority fields like renewable energies or micro/nano electronics. After a brief introduction to the high throughput modeling philosophy, and some prior research in several fields, I will discuss how the high throughput approach has been applied to the search of novel materials for thermoelectric energy conversion. We have concentrated on half Heusler compounds. Our search through 79,057 different compositions has yielded 75 thermodynamically stable ternary compounds. We have calculated the bulk thermal conductivity for these compounds, employing a fully ab-initio approach. We find a considerable fraction of compounds for which the bulk thermal conductivities are much lower than those of known half Heuslers. We have also developed several machine learning techniques that considerably reduce the computation time, while still yielding efficient screening. We have also estimated the thermoelectric figure of merit (ZT) of the compounds within the small grain approximation. When compared with common semiconductors like Si, Ge, or the III-V compounds, half-Heuslers stand out due to having higher power factors. Estimated ZT's suggest that for some of the nanograined half-Heuslers the figure of merit might reach values above 2.

NanoPhononics for Thermal Management

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The efficiency of today's thermal interface materials and nanoelectronic devices rely on the thermal properties of nanostructures. The governing mechanisms at play are related to phonon scattering at interfaces as for instance in layered systems or nano-object composites. Actual theoretical models however disagree with Kapitza resistance measurements by several orders of magnitude and very few data have been reported to define heat flux at a single nanocontact.

We will propose a new approach to the estimation of the interfacial contact resistance based on atomic scale simulations, which have been applied to carbon based thermal interface materials.

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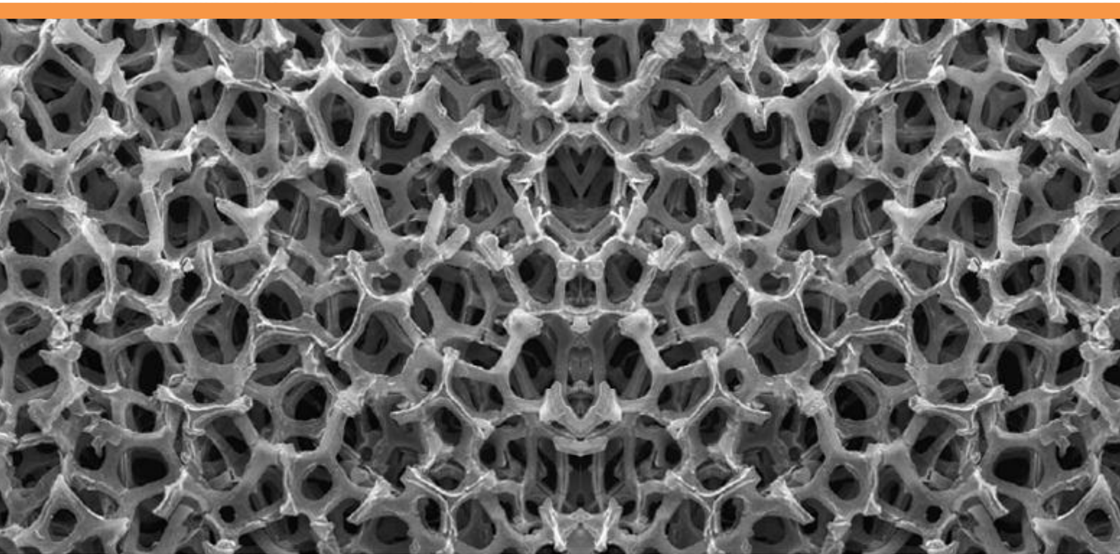

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