THIRD WORKSHOP ON PHONONS AND FLUCTUATIONS

21-24 May 2012, Sant Feliu de Guixols, Girona, Spain

Summary

The event was the third in a series of workshops focusing on topics related to phonons, nanophononics, fluctuations and local non-equilibrium. The previous workshops were held in Paris in November 2010 and September 2011. The workshop series has been arranged in close collaboration with the Group de Recherche (GDRE) on Thermal Nanosciences and Nanoengineering, Prof. Sebastian Volz, the Catalan Institute for Advances Researcher and Studies (ICREA), Prof Clivia Sotomayor Torres and VTT Technical Research Centre of Finland, Prof. Jouni Ahopelto.

The third workshop addressed issues such as heat transport in nanoscale systems, effects of phonon confinement, implications of phonons in biological systems and experimental techniques. One of the main aims was to strengthen the interplay between statistical physics and phononics.

65 participants from 11 countries attended the workshop. The organisers and part of the participants are active in coordination actions NANOTEC, nanoICT and NoE NANOFUNCTION, all funded by the European Commission and in the above mentioned GDRE. One of the targets of this series of workshops is to consolidate the field of phononics in Europe, the field that is becoming crucial for example for energy harvesting, thermal management, including nanoelectronics, optomechanical techniques and quantum compouting.

The presentations focused on the following areas: Statistical Physics, Theoretical and Experimental Approaches to Phononics, Phonons and Biology, Phonon Radiation, Confined Phonons and Nanometrology. The three day workshop consisted of 10 sessions with altogether 32 talks and two plenary talks, "Exciton coherence and decoherence in pigment protein complexes" by Susana Huelga, Ulm University, and "Phonons and photosynthetic energy transfer" by Greg Engel, University of Chicago. In addition, an excursion followed by a workshop dinner was organized in order to stimulate networking and encourage informal discussions among the participants.

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Scientific Contents

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Committees

Scientific Committee Members: Prof Dr Jouni Ahopelto (VTT Technical Research Centre of Finland), Prof Dr Clivia M Sotomayor Torres (Catalan Institute of Nanotechnology) Prof Dr Sebastian Volz (Ecole Centrale Paris)

Organising Committee: Ms Noemi Baruch (Catalan Institute of Nanotechnology) Dr Erwan Guillotel (Catalan Institute of Nanotechnology) Ms Ana de la Osa (Catalan Institute of Nanotechnology)

Support:

Ecole Centrale Paris, EU project NANOFUNCTION, European Science Foundation, Spanish Ministry of Economy and Competitiveness, CNRS Network Nanoscale/thermal, CEA, ICN, VTT.

In the following the scientific contents of the workshop is briefly described session by session.

Session 1: Statistical Physics

The first session was dedicated to stochastic statistical physics approaches to model the contribution of phonons to the heat transfer and conversion theme. Bart Cleuren (U Hasselt) described a new mechanism for refrigeration using photons to supply the power, elaborating on a thermodynamical description, to find the strong coupling regime needed for maximum cooling efficiency achieved by electron motion. The question of radiative heat transfer in nanostructures was addressed by Miguel Rubi (U Barcelona), who introduced a thermokinetic approach capable of fitting existing experimental results on radiative heat transfer across microgaps irrespective of geometrical configurations. The prospect of applying the model to phonon systems was also discussed. A recent view on the physical mechanism responsible for the Carnot limit of thermoelectric efficiency was presented by Giulio Casati (U Insubria at Como) based on dynamical non-linear models for thermopower. He discussed thermal rectification to control the heat current and showed that asymmetry plays a crucial but insufficient role, as it needs non-linearities. He discussed key issues, which urgently required a much deeper understanding of heat and charge transfer than currently achieved.

Session 2: Theory

In the first two talks given by Wu Li (LITEN-CEA) and Sebastian Volz (Ecole Centrale Paris), phonon transport was addressed based on two original approaches. The CEA team has developed a relaxation time equation to include terms beyond the single mean relaxation time approximation in the Boltzmann Transport Equation and the solving involves ab initio estimations of the equilibrium relaxation times. In the second talk, interfacial thermal resistance was derived according to a fluctuational model using the temperature as main quantity and several examples including polymer-Carbon Nanotubes (CNTs), Few Layer Graphene and CNT-silicon contact were presented. Finally, Jean-Luis Pichard (CEA-Saclay) talked about electronic quantum fluctuations that were computed based on a random matrix formalism to compute the quantum noise of the thermopower in model systems.

Session 3: Experimental 1

Jukka Pekola (Aalto University) discussed a small electronic system coupled to phonons, and debated that the classical fluctuation relations do not apply here and the effects arising from the evolution between the initial and final states should be included into relations. Christophe Blanc (CNRS-NEEL) described the behaviour of phonon transport in confined structures at low temperatures where the mean free path exceeds the physical dimensions, leading to trapping of phonons. The nonlinearities and the coupling of mechanical oscillation modes in suspended carbon nanotubes and graphene sheets were illustrated by Alexander Eichler (ICN). Very high Q-values and, consequently, high sensitivities can be achieved with these NEMS devices.

Session 4: Experimental 2

The important contribution of coherent acoustic phonons to the elasticity of nano-sized contacts and nano-composites, as well as to the heat flow across interfaces, was illustrated by Pascal Ruello (U Maine) based on recent work on colloidal materials. A drop of over a factor of 10 in the values of the elastic modulus with controlled decrease of the chemical bonds was demonstrated and the experimental methodology extensively discussed. The experimental technique is expected to provide measurements of surface energies of nanoparticles. Thomas Dekorsy (U Konstanz) reported on ways to study experimentally mechanical excitations close to the quantum limit with the contactless method of asynchronous optical pumping. The experimental results concerning scanning thermal probes for metrology at the nano-scale were presented by Stephan Dilhaire (LOMA, Bordeaux), who highlighted methodology and accuracy in temperature and spatial resolution.

Session 5: Phonons and Biology

This session consisted of two plenary talks. Susana Huelga (Ulm University) covered theoretically an interesting issue of quantum effects in biology, i.e., how can coherence survive in a noisy, wet and hot environment. One explanation is that noise creates transport paths that are otherwise forbidden and suppresses dephasing. It is obvious that biological entities exploiting noise to sustain coherence has the property to always use the most efficient coherent paths to transfer energy. Even phonon antennae are developed to harvest noise. Greg Engel (University of Chicago) talked about experimental work on phonon assited

photosynthesis. He has investigated the photoresponse of the Fenna-Mathew Olson complex of green sulphur bacteria using extremely fast optical methods with time resolution down to 4 fs. The quantum beats measured in the system sustain hundreds of ns even at room temperature. The protein's interaction with the quantum states in the FMO complex is nonspecific and allows reversible sampling of the states in the complex, leading to very high efficiency at elevated temperatures.

Session 6: Phonon Radiation

The first part of the session targeted on near field radiation effects on (i) the tip-substrate interaction based on Finite Domain Time Domain direct simulations (David Lacroix, LEMTA), (ii) the directional and spectral emissivity of a multilayer system by using genetic algorithm optimization (Jérémie Drévillon, Institut P'-Poitiers), (iii) the exaltation of the heat flux in a gap when intercalating a third layer (Ricardo Messina, Institut d'Optique-Paris XI). The second part has addressed the thermal conductivity prediction of ZnO based on a Boltzmann model (Patrice Chantrenne, MATEIS, INSA Lyon) and finally, transient effects on phonon transport revealed frequency dependent thermal conductivities (Younes Ezzahri, Institut P'-Poitiers)

Session 7: Confined Phonons

The session on confined phonons was covered with new data and potential interpretations by three different existing models on phonon lifetimes in the text-book example of free-standing silicon membranes by John Cuffe (ICN). The quest for a better understanding was highlighted and the effects of non-linear anharmonic terms discussed. Jean-Michel Mestdagh (CNRS-CEA, Saclay) presented a survey of electronic and vibrational energy redistribution in excited atomic and molecular systems with many degrees of freedom. Of special interest was the discussion on anharmonic resonances and their implications in the dynamics of the problem as well as the molecular dynamics and the connection to bandwidth of spectroscopy. Phillippe Lecoeur (Institue de Electronique Foundamental, U Paris IX) addressed the issue of coupling of thermoelectric generators and discussed the environment impact on performance.

Session 8: Phonon Radiation

The three presentations have provided different insights in near field radiation effects with the estimation of acoustic phonon gap transmission based on a scattering matrix definition of the transmission (Mika Prunnila, VTT), the expression of the near field radiation thermal conductance in a gap based on the Landauer formalism (Karl Joulain, Institut P'-Poitiers) and finally, the use of multilayer systems to design the spectrum and directionality of the emitted power (Philippe Ben Abdallah, Institut d'Optique-Paris XI).

Session 9: Nanometrology/Optics

Guillaume Baffou (Institut Fresnel-Marseilles) talked about thermo-plasmonics, i.e., using metal nanoparticles as local source of heat and the potential use for example in cancer therapy or tomography. The use of temperature modulation in detecting biomolecules was discussed by Charlie Gosse (LPN). The method can be used for example for point mutation detection. Emmanuel Peronne (Institut des Nanosciences de Paris) talked about the emission of acoustic phonons from self-assembled quantum dots probed by femtosecond pump and probe techniques, leading potentially to coherent acoustic phonon source.

Session 10: Nanometrology and local probes

This last session covered several aspects of probe metrology for (i) the local thermal conductivity measurement with the 3-omega method of materials with property gradients (Michai Chirtoc, Grespi-Reims), (ii) the estimation of nanowire thermal conductivity based on the 3-omega method (Dilhaire, LOMA-Bordeaux), (iii) the measurement analysis of hand-made microthermocouples (Laurent Thiery, Femto-ST), (iv) effects of contact geometry on scanning thermal microscopy (Séverine Gomes, CETHIL-Lyon), and (v) fluorescent crystal based temperature measurements (Nathalie Trannoy, Grespi-Reims)

In addition to talks, a number of posters were presented, mainly by students, in the meeting. Altogether, very lively and fruitful discussions were going on throughout the workshop and ideas to increase collaboration between the groups were implanted.

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Assessment and Impact

One of the main aims of the workshop series is to strengthen the community working on nanophononics in Europe. The European Commission has started to support this field through projects such as NANOPACK and NANOPOWER and coordination actions nanoICT, NANO-TEC, ZEROPOWER and NANOFUNCTION. In France a national network was established on thermal properties at nanoscale. Bringing these activities together is an asset to Europe to understand and exploit nanoscale thermal phenomena for, for example, energy harvesting and thermal management in ICT. Another aim has been to join the forces of the groups in statistical physics and phononics, which is really needed to develop proper theory for thermal properties and heat transport in small structures. Regarding these targets, the third workshop was very successful. The number of participants increased from the about 50 in the previous meetings up to 65 coming from 11 countries, with a high number of students.

At the moment the field is lacking of experimental tools providing information from very small structures or volumes and about local non-equilibrium. Scanning thermal probes are being developed for high resolution characterisation but these tools have rather slow dynamical response. The fast pump and probe methods can reach the required time resolution for non-equilibrium phenomena but are lacking spatial resolution. Thus, new techniques are needed and for that the interaction between experimental and theory groups is fruitful. Very interesting new field is the role of phonons in biological systems, as shown in the two plenary talks. It is clear that we are just starting to understand the operation of the simple biological systems and can learn much from them. All in all, the meeting was very fruitful, covering different aspects of phononics. The reception and comments from the participants were very positive.

Using nowadays fabrication techniques one can realise structures and devices with dimensions of the order of acoustic phonon wavelengths. This allows, on one hand, to investigate the effects of confinement, interfaces and local fluctuations, and on the other hand, to exploit this knowhow in optimising the performance of devices and developing new approaches for sensors and information technology. The former include, for example, thermal management of integrated circuits and their packaging. The latter can lead to more efficient and smaller energy harvesting devices and, consequently, powering of autonomous sensor networks, facilitating approaches to the realisation of ambient intelligence applications. Combination of phononic and photonic crystals for optomechanical modulators is one option for high speed data processing. Eventually coherent quantum devices operating at elevated temperatures may become available following the operation of biological entities.

Thus, by advancing the research in the field of phononics, the Phonons and Fluctuations Workshops can have a strong impact in Europe with the aim to bring together the experimental and theoretical communities of phonon physics, heat transfer (mechanical) engineering, statistical physics, biology (fluctuations), nanoelectronics, and (solid-state) quantum communications to start with in a *focused research programme on heat control in the nanoscale* in the first instance and on, e.g., *harvesting fluctuations* as a follow-on or parallel focus.

PHONONS AND FLUCTUATIONS 3 WORKSHOP 21-24 May 2012,

Sant Feliu de Guixols, Girona, Spain

Program

Monday 21 May								
19.30-20.15 Registration								
20.15-21.15 Welcome reception, Clivia Sotomayor Torres, Catalan Institute of Nanotechnology, Barcelona;								
Sebastian Volz, Ecole Centrale Paris; Jouni Ahopelto, VTT Technical Research Centre of Finlan, Espoo.								
Tuesday 22 May								
09.30-11.00 Session 1, Statistical Physics . Chair person: Sebastian Volz, ECP								
09.30-10.00 Cooling by heating: refrigeration powered by photons, Bart Cleuren, University of Hasselt								
10.00-10.30 Thermokinetic approach for the radiative heat transfer problem in nanostructures, Miguel Rubi, University of Barcelona								
10.30-11.00 Dynamical models for thermopower, Giulio Casati, University of Insubria at Como								
11.00-11.30 Coffee Break								
11.30-13.00 Session 2: Theory. Chair person: Jouni Ahopelto, VTT								
11.30-12.00 Ab-initio investigation of phonon transport in nanomaterials, Wu Li, LITEN-CH-CEA								
12.00-12.30 Thermal Interface Resistance, Phonon Transmission and Fluctuations, Sebastian Volz, Ecole Centrale Paris								
12.30-13.00 Thermopower distribution of chaotic quantum dots, Jean-Louis Pichard, CEA-Saclay								
13.00-15.00 Lunch								
15.00-16.30 Session 3: Experimental 1. Chair person: Clivia M Sotomayor Torres								
15.00-15.30 Fluctuation relations in electron transport in the presence of coupling to phonons, Jukka Pekola, Aalto University								
15.30-16.00 Thermal phonon transport in corrugated silicon nanowires, Christophe Blanc, Institut Néel, Grenoble								
16.00-16.30 Nonlinearities in mechanical resonators made from nanotubes and grapheme, Alexander Eichler, Catalan Institute								
of Nanotechnology, Barcelona								
16.30-17.00 Coffee Break								
17.00-18.30 Session 4: Experimental 2. Chair person: Sebastian Volz, ECP								

17.00-17.30 Coherent acoustic phonons in colloidal materials: probing subnanometric interfaces properties, Pascal Ruello, IMMM,

Université du Maine

17.30-18.00 Coherent acoustic excitation of multilayers and single nanostructures, Thomas Dekorsy, University of Konstanz

18.00-18.30 Thermal Metrology at the Nanoscale, Stephan Dilhaire, LOMA, Bordeaux

20.00 Dinner

Wednesday 23 May

09.00-10.30 Session 5: Phonons and Biology. Chair person: Jouni Ahopelto, VTT

09.00-09.45 Plenary talk: Exciton coherence and recoherence in pigment protein complexes: Susana Huelga, Ulm University

09.45-10.30 Plenary talk: Phonons and photosynthetic energy transfer, Greg Engel, University of Chicago

10.30-11.00 Coffee Break

11.00-12.40 Session 6: GDRE session. Phonons Radiation. Chair person: Clivia M Sotomayor Torres

11.00-11.20 Scattering of light by an AFM tip near a surface by FDTD and near-field to far-field transformation; Application to apertureless Scanning Near-field Optical Microscopy (a-SNOM), *David Lacroix, LEMTA, Nancy*

11.20-11.40 Selective emitters design and optimization for thermophotovoltaic applications, *Jérémie Drévillon, Institut P'-Poitiers*

11.40-12.00 Near-field heat transfer in three-body systems, Ricardo Messina, Institut d'Optique-Paris XI

12.00-12.20 Prediction of the Thermal Conductivity of ZnO Nanostructures, Patrice Chantrenne, MATEIS, INSA Lyon

12.20-12.40 Frequency Behavior and Shastry's Sum rule of the Dynamical Thermal Conductivity of Bulk Semiconductor Materials, Younes Ezzahri, Institut P'-Poitiers

12.40-14.30 Lunch

14.00-15.30 Session 7: Confined Phonons (90 mins). Chair person: Sebastian Volz, ECP

14.00-14.30 Lifetimes of confined phonons in free-standing silicon membranes, John Cuffe, Catalan Institute of Nanotechnology, Barcelona

14.30-15.00 Electronic and Vibrational Energy Redistribution in excited atomic and molecular systems with many degrees of freedom, Jean *Michel Mestdagh, CNRS-CEA, Saclay*

15.00-15.30 Coupling thermoelectric generator with environment impact on performances, *Phillippe Lecoeur, Institut d'Electronique Fondamentale – Université Paris XI*

17.00 Excursion and dinner

Thursday 24 May

09.00-10.20 Session 8: GDRE talks on Phonon Radiation. Chair person: Jouni Ahopelto, VTT

09.00-09.20 Acoustic Phonon Tunneling, Mika Prunnila, VTT Technical Research Centre of Finland

09.20-09.40 Tip-sample electromagnetic interaction in the infrared: Effective polarizabilities, retarded image dipole model and near- field

thermal, Karl Joulain, Institut P'-Poitiers

09.40-10.00. Near-field perfect emitter, Philippe Ben-Abdallah, Institut d'Optique-Paris XI

10.00-10.20 Anomalous IR-absorption resonances in confined dielectric with evidences of spatially non-local effects, Yann Chalopin, Ecole Centrale Paris

10.20-10.40 Coffee Break

10.40-12.00 Session 9: GDRE talks: Nanometrology/Optics. Chair person: Clivia M Sotomayor Torres

10.40-11.00 Temperature Imaging using Quantitative Phase Microscopy, Guillaume Baffou, Institut Fresnel-Marseilles

11.00-11.20 Heating in plasmonic nanostructures investigated by digital heterodyne holography, Gilles Tessier, Institut Langevin, Paris

11.20-11.40 Temperature modulation and quadrature video acquisition to selectively detect biomolecules in mixtures, Charlie Gosse, LPN

11.40-12.00 The origin of the emission of acoustic phonons in quantum dots systems after ultrafast optical excitation: Experimental facts and likely scenario, *Emmanuel Peronne, Institut des Nanosciences de Paris*

12.00-13.00 Lunch

13.00- 14.40 Session 10: GDRE talks: Nanometrology and local probes. Chair person: Sebastian Volz, ECP

13.00-13.20 Combined Scanning Thermal Microscopy, Photothermal Radiometry and 3omega Hot Wire Approaches to Heat Transport Characterization at Interfaces, *Michai Chirtoc, Grespi-Reims*

13.20-13.40 Optical and Thermal characterization of nanostructures by photothermal techniques, Roberto Livoti, University of Rome La Sapienza

13.40-14.00 Laurent Thierry, Femto-ST, Besançon

14.00-14.20 Contact metrologies for the investigation of the thermophysical properties of solid materials at the submicrometric scales, Séverine Gomes, CETHIL-Lyon

14.20-14.40 Calibration of temperature sensor based on the thermal-resistive probe with a photoluminescent microcrystal, NathalieTrannoy, *Grespi-Reims*

14.40-15.00 Workshop wrap-up and conclusion

15.00 Workshop end

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