SYMPOSIUM D

Phonons and fluctuations in low dimensional structures

Symposium Organizers:

Clivia M. Sotomayor Torres, ICREA and Catalan Institute of Nanoscience and Nanotechnology ICN2, Bellaterra (Barcelona), Spain

Sebastian Volz, Ecole Centrale Paris, Châtenay Malabry, France

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PROGRAM VIEW : 2014 Spring
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Symposium : D

Phonons and fluctuations in low dimensional structures

26 May 2014 | 27 May 2014 | 28 May 2014 | 29 May 2014

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start at	Subject	Num.
09:00	**Welcome and introduction to Symposium D - Clivia M Sotomayor Torres (ICN2)**	
	Nanoscale Thermal Transport I : Clivia M Sotomayor Torres (ICN2)	
09:15	**Ballistic and Coherent Phonon Heat Conduction in Bulk Materials and Nanostructures** **Authors :** Gang Chen **Affiliations :** Mechanical Engineering Department Massachusetts Institute of Technology Cambridge, MA 02139 USA **Resume :** Understanding phonon transport is important for many technological developments, examples are thermoelectric energy conversion, for which phonon heat conduction should be minimized, and thermal management of microelectronics, photonic devices, and batteries, for which heat conduction should be maximized. In this talk, I will start with a discussion of first-principles simulation on phonon heat conduction in bulk crystals, which reveals details on phonon scattering and mean free path distributions. I will explain the importance of resonant bonding on the low thermal conductivity of III-V semiconductors. I will then present a recently developed thermal conductivity spectroscopy technique to measure phonon mean free distribution and discuss experimental evidence on coherent contribution of phonons to heat conduction in superlattices, supported by detailed simulations. This material is based upon work supported as part of the "Solid State Solar-Thermal Energy Conversion Center (S3TEC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number: DE-SC0001299/DE-FG02-09ER46577.	D.1 1
	add to my program (close full abstract)	
09:45	**Nanostructured Ge:Mn thin film: an efficient thermoelectric material** **Authors :** Y. I. Liu, D. Tainoff, J. Richard, M. Boukhari, A. Barski, E. Hadji, A. Assy, S. Gomes, O. Bourgeois **Affiliations :** Univ. Grenoble Alpes, Inst. NEEL, F-38042 Grenoble, France CNRS, Inst. NEEL, F-38042 Grenoble, France Institut Nanosciences et Cryogénie, SP2M, CEA-UJF, 17 rue des martyrs, 38054 Grenoble, France CETHIL, 9 Rue de la Physique, INSA de Lyon, 69621 Villeurbanne, France **Resume :** With the development of nano-technologies, the domain of thermoelectricity is now intensely attracting researchers' attention. A new class of (nano-) material mentioned as "electron crystal – phonon glass" is expected to yield a well improved thermoelectric efficiency, which is characterized by the dimensionless figure of merit ZT ($ZT=S^2\sigma T/k$). Besides the fabrication of the nanomaterial, experimental challenges then lie in the accuracy of the measurements of the factors presented in the calculation of ZT: S (Seebeck coefficient), σ (electric conductivity) and k (thermal conductivity). Here we would like to present a highly promising germanium based thermoelectric material, along with the advanced experimental techniques developed for the characterization of its thermal properties. The material is a thin film of highly doped germanium matrix grown by Molecular Beam Epitaxy, which contains spherical nano-inclusions of Ge_3Mn_5 having tens of nanometers in diameter . These nano-inclusions are expected to inhibit the transport of phonons via scattering at nanoscale, while optimal electrical properties (S, σ) are maintained thanks to the high doping level and crystalline quality of the germanium matrix.	D.1 2

To confirm the thermoelectric properties of the material and to properly understand the physics of the involved phonon scattering mechanisms, we have developed a highly sensitive 3-omega technique for the measurement of thermal conductivity of these thin films. Initially proposed by D. Cahill in 1987 , the 3-omega method has, during the time, proved its great advantages in the measurement of thermal conductivity for thin films as well as for 2D nanostructured samples . Measurements carried out on several GeMn thin films have revealed a reduced thermal conductivity by a factor of 10 compared to the value of bulk Ge substrate. This reduction is tightly correlated to the microstructure of the thin film, i.e. the diameter, concentration and dispersion of the GeMn nanoclusters, parameters that can be deduced by TEM measurements. Similar results have also been found using a numerical simulation based on Maxwell-Boltzmann equation developed by Kim et al . Finally, the measurements of electrical conductivity and Seebeck coefficient lead to a ZT value of the thin film superior to 0.1 at room temperature. References: A. Jain et al, J. Appl. Phys., 109, 013911 (2011). D. G. Cahill and R. O. Pohl, Phys. Rev. B 35, 4067, 1987. M. Abdelhak SACI, Transport thermique dans les milieux nano-structurés (GaAs)n/(AlAs)n, Ph.D. thesis, 2011. A. Sikora et al, Rev. Sci. Instr., 83, 054902 (2012); Rev. Sci. Instrum. 84, 029901 (2013). W. Kim et al, J. Appl. Phys. 99, 084306 (2006)

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10:00 **Coffee break**

Phonons in Metrology and Biology : Gang Chen (MIT)

10:30 **Picosecond biophononics: application to single-cell biology**

Authors : Thomas Dehoux, Maroun Abi Ghanem, Omar F. Zouani, Marie-Christine Durrieu and Bertrand Audoin
Affiliations : Univ. Bordeaux, CNRS, UMR 5295, Institut de Mecanique et d'Ingenierie, Talence, France ; Univ. Bordeaux, CNRS, UMR 5295, Institut de Mecanique et d'Ingenierie, Talence, France

Resume : Cells have a complex composition that yields an intricate rheological behavior, appealing for measurements over a wide frequency range. However the existing techniques cannot exceed the kHz range, and rely for most on injected or contacting functionalized microprobes. Here, we use GHz acoustic phonons to probe the mechanical properties of single cells under physiological conditions. We culture animal cells on top of a biocompatible Ti metal film. Low-energy femtosecond laser pulses are focused at the bottom of the film to a micron spot to allow single-cell investigation. The subsequent ultrafast thermal expansion launches a longitudinal acoustic pulse in Ti, with a broad spectrum extending up to 200 GHz. The acoustic pulse is transmitted to the cell owing to the cell-Ti intimate contact. The phonon propagation in the cell is measured remotely with an ultrafast laser probe through Brillouin light scattering. This yields a direct measurement of the local stiffness and viscosity of cells. Simultaneously, the acoustic reflection coefficient at the Ti-cell interface is measured through the transient optical reflectance changes. Time-frequency analysis of the reflected acoustic pulses with a wavelet transform reveals an anomalous frequency dispersion of the acoustic reflection coefficient. This innovative technique offers a unique mean to investigate quantitatively cell-biomaterial interactions without fluorescent labels or mechanical contact to the cell.

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11:00 **Thermal transport and nanomechanics of nanoscale contacts in scanning thermal microscopy**

Authors : Oleg V. Kolosov, Manuel Pumarol, Benjamin J. Robinson
Affiliations : Physics Department, Lancaster University, Lancaster, LA1 3BE, UK

Resume : We experimentally explore one of the least defined areas in scanning thermal microscopy (SThM) – the thermal contact between the SThM probe tip and the studied sample by monitoring normal and shear forces between the nanoscale tip and the studied surface while measuring the heat transport from the tip. By using the measurements in both ambient and high vacuum (1x 10-7 Torr) environment we directly differentiate contributions of various channels of heat conduction in SThM. In order to measure in real-time the shear forces an SThM X-piezo was dithered creates a lateral sliding forces acting on the cantilever. The torsional and normal forces are both measured through and

D.2 2

recorded simultaneously with SThM signal. We found that the shear forces and thermal response are inversely correlated to the heat transport to the sample. Once the mechanical contact is established, our data both in air and vacuum, suggest that it is the solid-solid contact that is the dominant heat transfer channel of the thermal contact. If liquid bridge would be dominant, we should be able to observed significant decrease of the shear force, with the constant heat conduction that was not the case in our experiments suggesting that liquid bridge may be much less essential for nanoscale heat transport in SThM than generally accepted.

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11:15 **Heat transfer through the water meniscus at nanoscale contacts investigated with Scanning Thermal Microscopy** D.2 3

Authors : Ali ASSY*, Stéphane LEFEVRE, Pierre-Olivier CHAPUIS, Séverine GOMES
Affiliations : 1)Université de Lyon, CNRS 2)INSA-Lyon, CETHIL, UMR5008, F- 69621, Villeurbanne, France 3)Université Lyon 1, CETHIL, UMR5008, F-69621 Villeurbanne cedex, France

Resume : Scanning Thermal Microscopy (SThM) with its expected submicrometric spatial resolution is a promising tool to determine the local thermophysical properties of composite materials. Depending on experimental surrounding conditions, various heat transfer mechanisms may operate between the hot probe and the sample. These mechanisms must be better understood to optimize measurements. We focus in this work on the heat transfer through the water meniscus formed due to the capillary condensation of the ambient humidity. Because of the lack of information about it, this heat transfer is usually avoided in SThM. Here, we report on its contribution for various SThM probes and samples. The influence of the probe size is shown using probes of different sizes. Samples of hydrophilic and hydrophobic character are used to show the impact of the sample surface affinity to water on the probe/sample heat transfer. A correspondence in terms of variation depending on the probe temperature between the thermal signal and the capillary forces is evidenced. The meniscus thermal conductance is linked to the capillary forces based on theoretical models. The experimental results are compared with literature values. For each used probe, we introduce a model that takes into account all the heat transfer mechanisms that operate simultaneously between the probe and sample. The transposition of these results could be interesting for many related applications such as BioMEMS and NEMS/MEMS.

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11:30 **Optical and electrical thermometry of biased AlGaN/GaN HEMT structures** D.2 4

Authors : V.V. Strelchuk1, A.V. Naumov1, O.F. Kolomys1, A.S. Romanyuk1, S.A. Vitusevich2 and A.E. Belyaev1
Affiliations : 1. V. Lashkarev Institute of Semiconductor Physics of NASU, 03028 Kiev, Ukraine 2. Peter Grünberg Institute, Forschungszentrum Jülich, Jülich, Germany

Resume : In this work, we present the results of complex thermometry studies of AlGaN/GaN high-electron-mobility transistor (HEMT) structures using temperature-dependent Stokes and anti-Stokes Raman scattering and photoluminescence micro-spectroscopy together with electrical measurements. The thermal impedance and temperature rise of the 2DEG channel of biased AlGaN/GaN HEMT structures caused by the Joule self-heating have been determined by computer modeling and electrical measurements. In Raman measurements, from the analysis of intensities of Stokes and anti-Stokes signals and temperature dependence of the E2(high) phonon frequency shift, we determined the corresponding temperature of the 2DEG channel at different bias voltages. The temperature dependence of the Stokes Raman peak frequency and full width at half maximum (FWHM) of the E2(high) and A1(LO) phonon modes were analyzed by taking into account thermal expansion and phonon anharmonicity with the decay of optical phonons through the three and four-phonon processes. Temperatures derived from optical studies, electrical measurements and computer modeling are in good agreement.

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11:45 **A New Mechanism of Phononic Band Gap in Polymer Brush Particles** D.2 5

Authors : Elena Alonso-Redondo 1 Dirk Schneider 1 Michael Schmitt 2 Rebecca Sainidou 3 Pascal Rembert 3 Michael Bockstaller 2 Krzysztof Matyjaszewski 2 George Fytas 1,4
Affiliations : 1 Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany 2 Department of Materials Science and Engineering, Carnegie Mellon University, 5000 Forbes Avenue, 4307 Wean Hall, Pittsburgh 3 Groupe Ondes Acoustiques, Universite du Havre, Site Caucriauville, Pl. R. Schuman, BP 4006, 76610 Le Havre CEDEX, France 4 Department of Materials Science, University of Crete and IESL-FORTH, 71110 Heraklion, Greece

Resume : The convergence of complementary material properties results in the creation of a novel type of materials with a wide range of tunability. We report on the hypersonic phonon propagation in colloidal structures consisting of polystyrene (PS) polymer brushes grafted to silica hard spheres. The osmotic forces at the periphery of the particles are responsible for the spontaneous self-assembly during dropcast on a glass substrate and provide the opportunity to easily create colloidal crystal films. Using high resolution Brillouin light scattering the dispersion relation of their ordered structures and the vibration spectrum of the individual composite particles in air is recorded in the regime of high frequencies (GHz). The latter is necessary to assess possible hybridization-like band gaps in their ordered structures and to access the elastic properties of the PS brush coated silica cores. The star-like polymer topology is manifested on the two low frequency resolved modes which can be captured theoretically implementing imperfect boundary conditions at the SiO2-PS interface. For the ordered structures the experimental dispersion relation reveals a clear band gap in the vicinity of a flat band. Based on band structure calculations, these two new pertinent features, being different in colloidal crystals of hard spheres, are attributed to the hybridization of the particle eigenmodes with the effective medium acoustic bands of the crystal.

12:00 **Thermal probe for lipid bilayer study**

Authors : Jordane Soussi, Jeff Audiber, Bruno Le Pioufle, Olivier Français, Robert Pansu, Sebastian Volz, Yann Chalopin
Affiliations : Laboratoire EM2C SATIE, Institut d'Alembert, ENS Cachan PPSM, Institut d'Alembert, ENS Cachan

Resume : We present the use of a molecular rotor to investigate the thermal behaviour of lipid bilayers. The fluorescence lifetime of the rotor embedded in a suspended lipid bilayer is measured on a range of temperatures including the phase transition temperature. The fluorescence lifetime is correlated to the properties and behaviour of the lipid bilayer and the fluorophore, such as the phase of the membrane, using a Molecular Dynamics approach. This study seeks to use this rotor as a thermal probe for various experiments from protein localisation to thermal conductivity measurements in a lipid membrane.

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12:30 Lunch break

Electron-Phonon Interactions : Javier Rodriguez-Viejo (UAB)

14:00 **Evidence for a large phononic band gap leading to slow hot carrier thermalisation**

Authors : Simon Chung [1], Xiaoming Wen [1], Yu Feng [1], Neeti Gupta [1], Hongze Xia [1], Santosh Shrestha [1], Pyng Yu [2], Jau Tang [2], Gavin Conibeer [1]
Affiliations : [1] Australian Centre for Advanced Photovoltaics, University of New South Wales, Sydney, Australia [2] Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan

Resume : It has been proposed that the rate of hot carrier thermalisation can be slowed down if there is a sufficiently large gap in the phonon dispersion for a bulk material. This phenomenon is critical for the development of high efficiency hot carrier solar cells to minimise energy loss to thermalisation. A gap where the minimum of the optical branches is at least twice that of the maximum of the acoustic branches can prevent the primary pathway where optical phonons loses energy, the Klemens? decay mechanism. The large gap in the phonon dispersion eliminates the Klemens? decay pathway due to energy and momentum conservation laws. This enables the electron population to remain hot by allowing sufficient time for optical phonons to re-scatter its energy to electrons. Binary compounds with a large mass difference between the two constituent atoms and high level of crystal symmetry such as zirconium nitride and hafnium nitride (HfN) have such a gap in their phonon dispersion. HfN thin films have been sputtered on silicon and quartz substrates. Characterisation of hot electron lifetimes in HfN films have been performed using ultrafast transient absorption spectroscopy. Preliminary analysis of transient absorption data, both spectra and time evolution has indicated high carrier temperatures with a nanosecond long decay time. It is postulated the long hot carrier lifetime is due to the large phononic gap.

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14:30 **Effect of electron-phonon coupling on interfacial heat transfer**
Authors : S. Merabia, J. Lombard, F. Detcheverry
Affiliations : CNRS and Université Lyon 1
Resume : Despite decades of research, our understanding of interfacial thermal transport is still quite poor. Traditional models such as AMM and DMM fail to give a good description of the thermal boundary resistance between a metal and a dielectrics. In this contribution, I will discuss the effect of electron-phonon coupling in the value of the thermal boundary resistance between a metal and silicon or silica, using a combination of analytic approach and numerical simulations. I will analyze two applications: the thermal response of thin metallic films deposited on silicon or silica, and hyperthermia driven by core-shell nanoparticles.
D.3 2

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14:45 **Electron-Phonon Coupling Engineering for Thermal Devices**
Authors : M. Prunnila, D. Gunnarsson, J. Richardson-Bullock, M. J. Prest, T. E. Whall, E. H. C. Parker, L. Donetti, F. Gamiz
Affiliations : VTT Technical Research Centre of Finland; University of Warwick, UK; Universidad de Granada, Spain;
Resume : Operation of electron refrigerators and thermal detectors, such as bolometers, depends on the strength of the coupling of the electrons to the thermal bath. The coupling is, in the end, deter-mined by the thermal electron-phonon coupling (TEPC), i.e., the thermal conductance between the electron and phonon systems. TEPC depends strongly on the microscopic details of the system at hand. In semiconductors and also in graphene the coupling can be tuned, for example, by strain and by adjusting the carrier concentration. Strain-tuning of TEPC has been investigated theoretically and experimentally in many-valley systems [1,2] and applied in enhancing the performance of silicon based electron refrigerators [3]. However, the effect of strain on TEPC is orders of magnitude smaller than suggested by the theory. In this contribution, we discuss this discrepancy and other heat dissipation channels that can become dominant at very low temperatures. One possible channel is provided by the near-field electron-electron interaction between closely spaced conductors [4], which suggests that thermal management of low-temperature devices could possibly utilize near-field heat transfer even in the case of solid-solid contact. References: [1] M. Prunnila, Phys. Rev. B 75, 165322 (2007). [2] J.T. Muhonen et al. Appl. Phys. Lett. 98, 182103 (2011). [3] M.J. Prest et al., Appl. Phys. Lett. 99, 251908 (2011). [4] M. Prunnila and S. Laakso, New J. Phys, 15 033043 (2013).
D.3 3

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15:00 **Acoustic gain in piezoelectric semiconductors at epsilon-near-zero response**
Authors : Johan Christensen Morten Willatzen
Affiliations : DTU Denmark
Resume : We demonstrate strong acoustic gain in electric-field biased piezoelectric semiconductors at frequencies near the plasmon frequency in the THz range. When the electron drift velocity produced by an external electric field is higher than the speed of sound, Cherenkov radiation of phonons leads to amplification of sound. It is demonstrated that this effect is particularly effective at epsilon-near-zero response leading to giant levels of acoustic gain. Operating at conditions with strong acoustic amplification, we predict unprecedented enhancement of the scattered sound field radiated from an electrically controlled piezoelectric slab-waveguide. This extreme sound field enhancement in an active piezo material shows potential for acoustic sensing and loss compensation in metamaterials and nonlinear devices [1]. [1] Phys. Rev. B. Rap. Comm. (accepted 2014)
D.3 4

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15:15 **Experimental determination of the vibrational density of states in metallic nanocrystals**
Authors : Maxime Bayle, Patrick Benzo, Nicolas Combe, Christophe Gatel, Caroline Bonafos, Gérard Benassayag, Robert Carles
Affiliations : CEMES/CNRS - Université de Toulouse, 29 rue Jeanne Marvig 31400 Toulouse, France
Resume : Investigating the dynamical properties and particularly the electron-phonon interactions at the nanoscale is of prime interest for all the applications exploiting thermodynamics effects in low dimensional structures. In this work, we show how a detailed image of the entire vibrational density of states (VDOS) in metallic nanocrystals is obtained using Raman scattering. A specific sample architecture, set-up configuration and original elaboration process are used to
D.3 5

take advantage of spectrally and spatially localized surface plasmon resonance, optical amplification and dark-field spectroscopy, simultaneously. Disentangling the atomic vibrational contribution and electron-hole excitation (i.e. the so-called "background" in SERS) is performed. This procedure is applied to colloidal gold nanocrystals deposited on a surface, and to silver nanocrystals embedded in a dielectric matrix. The extracted VDOS is successfully compared with theoretical ones obtained by atomic scale simulations. The effects of confinement, surface, disorder and strain on the VDOS are discussed. In particular, the strain effect is investigated experimentally using the geometrical phase analysis coupled with high-resolution transmission electron microscopy.

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15:30 **Coffee break**

Poster Session I : Sebastian Volz (ECP)

16:00 **Phonon decay in silicon nanocrystals: fast phonon recycling**
Authors : A. A. Prokofiev, A. N. Poddubny, and I.N. Yassievich
Affiliations : Ioffe Physical-Technical Institute of the Russian Academy of Sciences, 194021 St. Petersburg, Russia
Resume : A theory of electron-phonon interaction and phonon decay in Si nanocrystals based on sp3d5s* empirical tight-binding model and anharmonic Keating model is presented. It is demonstrated that the time of optical phonon emission by hot carriers in Si nanocrystal lies on subpicosecond time scale. However, the fast phonon recycling should decrease the energy relaxation rate of carriers excited in Si nanocrystals. Phonon recycling process stops only after the anharmonic decay of high-energy phonons into the lower energy ones. This low energy acoustic-like phonons can relatively easy leave the nanocrystal, so the energy of the system ?carriers phonons" is dissipated. Thus, the energy relaxation rate is governed not just by the phonon emission rate, but also by the optical phonon decay rate. The decay rate of the optical phonon into the two phonons of smaller energy is found to be in the range of 1 to 10 ps. It is demonstrated by applying Monte-Carlo simulation that the phonon recycling decreases the rate of energy relaxation for hot electrons localized in Si nanocrystals [1]. [1]. A.A. Prokofiev, A.N. Poddubny, I.N. Yassievich, arXiv:1304.1623. D.P.12

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16:00 **Thermal conductivity of modulated Bi2Te3 nanowires**
Authors : Konstantinos TERMENTZIDIS and David LACROIX
Affiliations : LEMTA, CNRS UMR-7563, University of Lorraine, Vandoeuvre les Nancy, France
Resume : The reduction of the thermal conductivity of nanostructured materials is of great interest for almost all devices and crucial for the thermoelectric efficiency. The development of new fabrication methods allows tailoring nanostructured materials and their transport properties. Bulk Bismuth Telluride is the most efficient thermoelectric material near room temperature. Bi2Te3 nanowires are of particular interest as they are inexpensive to be fabricated (electrochemical deposition) and their reduced thermal conductivity due to the lower dimension can be lowered further with structural modulation. Important parameters that can change the transport properties are the stoichiometry, the roughness of the external surfaces, the state of the interfaces in the case of core/shell type nanowires, as well as the doping. With means of molecular dynamics and using realistic potential, we predict the thermal conductivity of a series of modulated Bi2Te3 nanowires. We will prove that the roughness provides efficient scattering across a broad spectra of phonons, and can reduce the thermal conductivity close to the amorphous limit. D.P.13

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16:00 **Phonon dispersion relations of Sb2S3 and Bi2S3 using the supercell force-constant method**
Authors : C. K. Gan [a], K. T. E. Chua [b], and Y. Liu [a]
Affiliations : [a] Institute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632. [b] Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA. D.P.14
Resume : We present a lattice dynamical study on the orthorhombic antimony sulphide (Sb2S3) [1] and bismuth sulphide (Bi2S3) [2] using the supercell force -constant method. We find that the slow decay of the interatomic force

constants for these compounds in the Pnma setting requires the use of a large supercell of 2 x 4 x 2 that consists of 320 atoms. To enable a practical calculation the space group information is fully utilized where only inequivalent atoms within the primitive cell are displaced for the force calculations. The effect of Born effective charges is incorporated into the method. We compare our results with that obtained from the density-functional perturbation theory. We found that smaller supercells could lead to unphysical acoustic phonon softening and lifting of the degeneracies along high symmetry directions. Our results serve to suggest that for a proper use of the supercell force-constant method, the supercell size has to be tested along with other parameters such as the kinetic energy cutoff, the Brillouin zone sampling or the self-consistent convergence criteria. [1] Y.Liu, K.T.E. Chua, T.C. Sum, and C.K. Gan, PCCP 16 (2014) 345. [2] Y. Zhao, K.T.E. Chua, C.K. Gan, J. Zhang, B. Peng, Z. Peng, and Q. Xiong, Phys. Rev. B 84 (2011) 205330.

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16:00 **Studies of surface optical phonons based on GaN and ZnO nanostructures prepared with “top down” method**

Authors : X. H. Wang, S. J. Xu
Affiliations : Department of Physics and HKU-Shenzhen Institute of Research and Innovation (HKU-SIRI), The University of Hong Kong, Pokfulam Road, Hong Kong, China

Resume : Surface vibration modes in small solids have received great interests in the past decades. Currently, various nanostructures and nanometerials with huge surface-to-volume ratios offer an excellent platform to study surface vibrations and great chance to verify some theoretical modifications on the classical phonon theories for large crystals. Originated from the Lyddane-Sachs-Teller relation which describes the relationship between the transverse optical (TO) and longitudinal optical (LO) modes in crystals, surface optical (SO) phonon mode was predicated with a frequency lying in between the TO and LO modes. The observations of SO phonons have been reported in semiconductor nanostructures such as nanowires and nanospheres etc. However, the SO phonons discussed in the previous reports fall in two different categories: one model considers individual nanostructures as an isolated object and SO phonon frequency is related to its geometric features such as shape and size while the other believes that phonon frequency is highly associated with the nanostructures’ density or filling factor rather than its geometry. So far most of the reported experimental studies were based on nanostructures fabricated by “bottom up” approach. In these samples concentration and uniformity of nanostructures could not be accurately controlled. Meanwhile, the signals recorded in most of the previous studies were actually from many nanostructures. In the present study, we conduct a systemic study of SO phonons based on GaN nanostructures fabricated by focused ion beam (FIB) milling. The focused beam of high-density ions bombards the sample with high precision according to the preset digital mask which offers great flexibility in structural dimension and density. GaN nanostrips and nanopillars with various dimensions were fabricated and optically characterized by a WITec scanning confocal Raman microscopy. Meanwhile, FIB fabricated ZnO nanostructures were also investigated for a comparative study. Preliminary Raman results for the SO phonons show a good consistency in these two systems and detailed systematic results will be presented.

D.P.15

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16:00 **Ballistic-diffusive heat conduction equations in 1D and 2D geometries**

Authors : Pierre-Olivier CHAPUIS, Yunxin WANG, Nabil DJATI
Affiliations : Centre for Thermal Sciences, Lyon (CETHIL) CNRS - INSA Lyon - UCBL Campus La Doua - LyonTech 69621 Villeurbanne (Lyon), France

Resume : The Boltzmann transport equation (BTE) allows simulating heat transfer when the characteristic dimensions of the medium start to be comparable to the heat carrier mean free paths. However, the equation is not straightforward to solve and it can be useful to consider approximated equations. The ballistic-diffusive heat conduction equations (BDE) have been proposed as a tool to simulate heat transfer in subdiffusive configurations. Our aim is to investigate their advantages and drawbacks. We analyze the results of phonon simulations with the BDE in monodimensional and bidimensional geometries for grey media, where heat carriers possess a single mean free path, and non-grey media. The goal is to split the effect of confinement and dispersion. The 1D case is simple and it is verified that the results can be approximated with a simple analytical equation. The 2D case is analyzed based on the information got from the previous analyses. It is shown that care should be taken close to the boundaries. We discuss the results obtained with a heat

D.P.16

source with size comparable with the mean free path, useful for many experiments involving thermal constrictions.

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16:00 **Thermally-Active Screw Dislocations in Si Nanowires and Nanotubes**

Authors : Shiyun Xiong1, Jihong Ma2, Sebastian Volz1, and Traian Dumitrică2
Affiliations : 1 EM2C UPR CNRS 288 École Centrale du Paris, 92295 Châtenay-Malabry, France 2 Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, USA

Resume : New properties appear when nanomaterials contain dislocations. Understandings whether these features, which arise naturally during growth, are beneficial or problematic becomes essential for developing applications. Here we investigate <110> Si nanowire and nanotube structures containing an axial screw dislocation, as described by objective molecular dynamics coupled with the classical Tersoff potential. By means of direct nonequilibrium molecular dynamics simulations, we uncover a decrease in thermal conductivity in the presence of axial screw dislocations with closed and open cores. Analysis based on the atomistic Green function method reveals that this decrease originates in the phonon-phonon scattering due to the anharmonicity introduced especially by the highly distorted core region. As high-strain is intrinsic to dislocations, the effect should occur to various extents in other nano-materials.

D.P.17

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16:00 **Thermal conductivity of single DLC nanowire**

Authors : L. Jalabert(1), T. Sato(2), G. Valet(2), D. Guo(3), R. Kometani(3), H. Fujita (2), S. Volz(4)
Affiliations : (1) LIMMS-CNRS/IIS-University of Tokyo, Japan (2) IIS, Univ. of Tokyo, Japan (3) Grad. Sch. of Eng., Univ. of Tokyo, Tokyo, Japan (4) LEM2C, Ecole Centrale Paris, Paris, France

Resume : Diamond, which has the best bulk thermal conductivity, is an excellent candidate for heat dissipation issues in the micro-nanodevices industry. Whereas diamond thin films are already used in nano-electronics, there are several engineering challenges appearing in the fabrication of 1D diamond wires. Ab-initio simulations showed larger size dependence compared to Si-NW [1], which is very interesting to create heat dissipation bridges for MEMS and nano-devices. However, there is still a lack of experimental measurement of thermal properties of individual diamond nanowires. Here, we measured the thermal conductivity of a single diamond-like carbon nanowire (DLC-NW) bridged between a micro-heater and a temperature sensor. DLC-NW of 1mic in length and 85nm in diameter is fabricated by FIB-CVD with an excellent adhesion and mechanical strength [2]. A new TEM cryogenic holder was developed to conduct electrical measurements on MEMS at low temperatures in UHV. The MEMS temperature sensor is made of Cr/Pt/Al and connected to an external AC Wheastone bridge while DC pulses are supplied on a micro-heater. The thermal conductivity was measured around 200 W/m.K between 250K and 350K. The values are lower than in reported simulations for a pure diamond nanowire with diameter of 50nm [1] probably due to the amorphous structure of DLC, but still very promising for heat management applications. [1] W. Li, et al, Phys. Rev. B 85, 195436 (2012). [2] D. Guo et al, JJAP, Vol. 51, 065001, (2012).

D.P.18

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16:00 **Effect of Substrates on the Thermal Conductivity of Silicene**

Authors : Xiaoliang Zhang1; Ming Hu1,2
Affiliations : 1 Institute of Mineral Engineering, Division of Materials Science and Engineering, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52064 Aachen, Germany; 2 Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, 52062 Aachen, Germany

Resume : Silicene, the silicon-based counterpart of graphene with a two-dimensional honeycomb lattice, has been attracting tremendous interest both theoretically and experimentally due to its significant potential industrial applications. Even though free-standing silicene has supreme physical and chemical properties, it's not easy to fabricate and most of the existing silicene are grown on various substrates. Therefore, it's of great importance to investigate the substrate effect on the physical and chemical properties of silicene. First-principles calculations have shown great effect of substrates on the electronic properties of silicene. Except electronic properties, the substrate effect on the thermal transport properties of silicene is also very worthy to study due to potential thermal management applications of silicene. By conducting a series of non-equilibrium molecular dynamics simulations, we show that

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substrates have great effect on the thermal conductivity of silicene. More importantly, substrates can tune the thermal conductivity of silicene in a broad range, which is very important for the thermal management of electronic devices involving silicene. By phonon-related analysis, a mechanism for the substrate effect, which is fundamentally different from that for supported graphene, is clearly identified. Our work provides deep insights for understanding the underlying mechanisms of thermal transport in supported silicene, which will be helpful for the design of silicene-based electronic devices.

add to my program (close full abstract)

16:00 **Determination of thermal conductivity in (nanostructured) SiGe materials**

Authors : Konstanze Hahn, Claudio Melis, Luciano Colombo
Affiliations : Department of Physics, University of Cagliari

Resume : Thermoelectric energy production has recently gained increased interest as an alternative energy resource accompanied by the quest for materials with enhanced thermoelectric properties. However, optimization of the efficiency of such materials is not trivial since the integrated parameters (Seebeck coefficient, electrical and thermal conductivity) are interdepending properties. In this respect, SiGe-based materials have recently been found to be promising candidates. Here, we have investigated the effects of structural changes of various SiGe-based materials, namely SiGe bulk alloys, nanocrystalline and amorphous SiGe on their thermal conductivity. The thermal conductivity has been calculated by means of the so-called approach-to-equilibrium molecular dynamics where the thermal conductivity is estimated by the temperature evolution in the transient regime. With this method it is not required to reach thermal equilibrium thus significantly reducing the computational cost compared to other methods such as Green-Kubo or direct methods.Thermal conductivity in SiGe bulk alloys is reduced remarkably already at very small contents of Ge and Si compared to the pure crystalline Si and Ge, respectively, and could be further decreased in nanocrystalline SiGe. Even lower values of the thermal conductivity have been found in amorphous SiGe. Based on these results it is proposed that amorphous SiGe exhibits enhanced thermoelectric properties compared to bulk alloy or nanocrystalline SiGe.

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add to my program (close full abstract)

16:00 **Study of thermal transport in hydrogenated graphene by non-equilibrium molecular dynamics.**

Authors : Giuliana Barbarino, Claudio Melis, Luciano Colombo
Affiliations : Department of Physics - University of Cagliari

Resume : Graphene can react with atomic hydrogen, creating a stable material which retains its crystalline hexagonal lattice, called Graphane. Graphane can experimentally synthesized by exposing suspended Graphene to hydrogen plasma [D. C. Elias et al., Science 323,610 (2009)]. While it has been recently shown that Graphane structural and electronic properties strongly differ from pristine Graphene, no estimate are available concerning its thermal transport coefficient. In this work, we obtain the first prediction ever done of Graphane thermal conductivity in three different isomers (B,C and W) by using the novel approach to equilibrium molecular dynamics (AEMD) technique [E. Lampin et. al., J. Appl. Phys.,114, 033525 (2013), C. Melis et al.,s Phys. Rev. B]. The calculations have been performed using the reactive empirical bond order potential implemented in LAMMPS code. For all the three isomers we estimate a thermal conductivity value significantly lower than the pristine Graphene one. We attribute such a behavior to the sp2-sp3 hybridization change, taking place upon Graphene hydrogenation. In all the three samples, thermal transport is showed to be little anisotropic with respect to the armchair and zig-zag directions . The following results suggest that hydrogenation can be a way of tuning Graphene thermal conductivity and managing heat dissipation in graphene nanoelectronics devices.

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16:00 **Monte Carlo simulations of phonon transport in porous semiconducting nanostructures**

Authors : V. JEAN, S. FUMERON, K. TERMENTZIDIS, D. LACROIX
Affiliations : Université de Lorraine, LEMTA, CNRS-UR 7563, BP 70239, 54506 Vandoeuvre Cedex, France

Resume : Tuning the thermal conductivity (TC) through the engineering of phonon scattering processes in nanostructured semiconductors is a promising way to improve their thermoelectric properties. Phonon wave-guides, phononic crystals as well as nano-porous media have already demonstrated their ability to reduce the TC and control the phonon heat flux. This study is performed in this framework and focuses on phonon scattering induced by pores, in structures like

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nanowires and nanofilms, for various sizes, shapes and pore's spatial organization. In semiconductors, the pore occurrence induces a "boundary-like" scattering process that can be evaluated thanks to a "porous mean free path" (pMFP). This parameter is first computed with a ray-tracing method, which has proven to be very efficient for several pore geometries. Then, pMFP is implemented into an Effective Monte Carlo simulation tool (EMC) to assess the TC of porous nanostructures through the resolution of the Boltzmann transport equation. Among the studied parameters, we focused on the influence of the pore: size, shape (cubic, spherical and ellipsoidal) and organization (aligned, staggered, random and graded distributions) for the pMFP appraisal and TC calculations. Our Monte Carlo simulations show that TC can be reduced by two orders of magnitude, even at low porosity. We also point out that a diffusive regime can be recovered for highly scattering nanostructures, even if their characteristic length is below the bulk limit.

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16:00 **Vacuum phonon tunneling through Casimir force between two solid materials**

Authors : YOUNES EZZAHRI and KARL JOULAIN
Affiliations : Institut Pprime, Université de Poitiers-CNRS-ENSMA 2, Rue Pierre Brousse Bâtiment B25, TSA 41105 86073 Poitiers Cedex 9 France

Resume : Understanding and controlling heat transfer at very short length scales, has become very crucial in the last decade due to the continuous development in nanotechnology and the rapid evolution in the synthesis and fabrication of different materials at a nanometer scale. At these scales, two heat transfer mechanisms become dominant, namely near field radiation and interface conduction between two solid materials. As the distance between the two latter decreases, there will be a natural transition from the radiative regime to the conductive regime of heat transfer when the two solids are in contact. The aim of the present work is to shed light on this specific transition by investigating the possibility of phonon tunneling in vacuum through Casimir force between the two solids. We analyze how this mechanism of heat transfer compares and competes with the near field radiation using a nonlocal model of the dielectric function. We show that the former mechanism can be very effective and even overpass the latter mechanism depending on the nature of the solid materials, the distance gap between them as well as the operating temperature regime.

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16:00 **Phonon Fano Antiresonances in Nanostructures with Embedded Planar Defect-Atom Arrays**

Authors : Haoxue Han, Yuriy A. Kosevich, Sebastian Volz
Affiliations : Laboratoire d'Energetique, Moleculaire, Macroscopic et Combustion, CNRS UPR 288, Ecole Centrale Paris, Chatenay-Malabry 92295, France

Resume : Recent progresses in the field of thermoelectric materials have clearly uncovered the substantial gain obtained from the decrease of thermal conductivity. Exploring new alternatives to introduce additional thermal barriers in solid and crystalline materials is hence of primary importance. We propose to exploit a new physical mechanism based on phonon Fano antiresonance to manipulate the thermal phonon distribution in crystals. By introducing planar and periodic defect-atom arrays, phonons are led into both a non-defective and a defective paths. The resulting destructive interference of the waves generates a stop band in the thermal phonon spectrum that can be controlled by the mass of the defect atoms. We use both analytical and Molecular Dynamics technique to investigate this phenomenon and design the optimal configuration. A Wave-packet Dynamics technique is implemented to provide a per-mode transmission and highlight the heat carrier spectrum with respect to the defect masses. The results are then confronted to a lattice dynamic approach for confirmation.

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16:00 **Phonon Blocking in Multilayers produced by Pulsed Laser Deposition**

Authors : F. Döring, C. Eberl, A.Major, S. Schlenkrich, F. Schlenkrich, M. Lüttich, M. Mansurova, B. Lenk,S. Hoffmann, M. Münzenberg and H. U. Krebs
Affiliations : Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany; 1st Institute of Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany; Institute for x-ray physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

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Resume : Multilayer insulations are a modern high-technology approach for minimizing thermal transport, which is important for thermoelectric materials, thermal barrier coatings, solid state refridgerators and cryogenic applications. In these multilayer structures, the thermal conductivity can be reduced by an increasing number of interfaces between two materials with a high acoustic

mismatch resulting in different phonon dispersion relations. Therefore, different types of multilayers, consisting of various metals (e.g. W, Ti, or Cu), oxides (e.g. ZrO2 or MgO) and polymers (e.g. PC), were selected and pulsed laser deposited (PLD at 248 nm) with high quality and afterwards analysed by ultrafast pump-probe reflectivity measurements. Thereby we found fast phonon modes on ps time scales that indicate possible candidates for THz frequency band gap phononic metamaterials. In this contribution, the necessary steps for the fabrication of phononic metamaterials by PLD and first results of reflectivity measurements are discussed.

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16:00 **Coherent Electron Transfer in Polyacetylene**
Authors : Demetra Psiachos
Affiliations : University of Crete
Resume : We examine, using a mixed classical-quantum electron-ion dynamics model, electron transfer in a donor-acceptor-like molecular junction system based on polyacetylene. We identify two qualitatively-different transfer regimes: hopping and tunnelling. We discuss the criteria for achieving each one and for minimizing inelastic scattering and decoherence arising from the coupling to the ions, and we connect our main results to quantities derived from electron dynamics in simpler, three-state model systems. We identify the requirements to have near-ballistic transfer and discuss our predictions in the context of recent experimental results. D.P.116

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16:00 **Thermal conductivity of AlN crystals with oxygen impurities: A Molecular Dynamics Study**
Authors : Wassim KASSEM, Juliana JARAMILLO-FERNANDEZ, Sebastian VOLZ, Yann CHALOPIN, Emmanuel OLLIER, Michel KAZAN
Affiliations : EM2C, CNRS UPR 288 Ecole Centrale Paris, Chatenay-Malabry; LITEN, CEA, Grenoble; Department of Physics, AUB, Beirut
Resume : The thermal conductivity of polycrystalline aluminum nitride films is known to be highly affected by the concentration of oxygen atoms present due to the manufacturing process. The decrease in thermal conductivity is due to the shorter mean free path of phonons scattered by the impurities. In this work we present experimental results describing how the oxygen atoms are incorporated into the AlN lattice using FTIR measurments, and show the dependence of this on temperature. We compare the phonon properties of the impregnated samples to molecular dynamics simulations, and we present a study of the thermal conductivity of the simulated AlN crystal using MD. D.P.117

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16:00 **Surface acoustic wave bandgaps for conical pillars on a piezoelectric substrate**
Authors : A. Mrabti1, M. Oudich1, A. Akjouj1, Y. Pennec1, B. Djafari-Rouhani1, A Talbi,2 J. Streque2, Y. Du2, A. Soltani2, P. Pernod2
Affiliations : 1IEMN, UMR CNRS 8520, Université de Lille 1, 59655 Villeneuve d'Ascq ; 2LIA LEMAC, IEMN, UMR 8520,ECLille, Université de Lille 1, 59655 Villeneuve d'Ascq
Resume : We report theoretically on the band structure of a square lattice phononic crystal made up of nickel (Ni) conical pillars deposited on the surface of a semi-infinite LiNbO3 substrate. Calculations have been performed with a 3D finite element method taking into account material anisotropy and piezoelectricity of the LiNbO3. We demonstrate the existence of wide surface acoustic wave (SAW) bandgaps determined from the band structure. The effects of pillar geometry on the existence of large surface acoustic bandgaps are investigated. The structure is realized experimentally and transmission and phase time curves show a good agreement with our theoretical calculation. We investigate further the effect of the geometrical parameters on the behavior of the lowest SAW bandgap, by changing the height h and radius r of the pillars as well as the angle □ of the cone. When increasing h, the band gap frequency shifts downwards and slightly widens. The band gap can be significantly widened by decreasing the radius r. Finally, by increasing the angle □ of the cone, the gap shifts downwards and increases its width. D.P.118

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16:00 **Covalent Bond-induced thermal transport enhancement at graphene nanoarchitectures**
Authors : Xiangjun Liu, Gang Zhang, Yong-Wei Zhang
Affiliations : Institute of High Performance Computing, A-STAR, Singapore; Institute of High Performance Computing, A-STAR, Singapore; Institute of High Performance Computing, A-STAR, Singapore D.P.119

Resume : Tailoring interfacial thermal transport in graphene-based nanoarchitectures is important for many applications including nanoelectronics, solid-state lighting, energy generation and nanocomposites. We demonstrate that interfacial thermal conductance G can be fivefold enhanced by introducing covalent bonds at the interfaces using molecular dynamics simulations. The simulations captured the trend of thermal transport enhancement with the increment of interfacial covalent bond density. The results confirm that the observed G enhancements at the interfaces are due to strong interfacial covalent bonds and resultant coupling in the atomic vibrational spectra near the interface. The spectral analysis indicates that the coupling between graphene out-of-plane motion and bonded linkage group motion at low frequencies serves as the most important channels for thermal transport across the interface. Thus, covalently bonding functionalization is an attractive approach to tune the heterointerfacial thermal transport in a variety of material systems.

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16:00 **Time Domain Thermoreflectance Measurements of Gold – (Gallium Oxide) – Gallium Nitride Interfaces as a Function of Surface Roughness**

Authors : Chester Szwejkowski [1], Kai Sun [2], Costel Constantin [1], Ashutosh Giri [3], Christopher Saltonstall [3], Patrick E. Hopkins [3]
Affiliations : [1] Department of Physics and Astronomy, James Madison University, Harrisonburg, Virginia USA; [2] Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan USA; [3] Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia USA

Resume : Gallium nitride (GaN) is considered the most important semiconductor after the discovery of Silicon. Understanding the properties of GaN is important in determining the utility and applicability of this class of materials to devices. We present results of time domain thermoreflectance (TDTR) measurements as a function of surface root mean square (RMS) roughness. We used commercially available 5mm x 5mm, single-side polished GaN (3-7 μm)/Sapphire (430 μm) substrates that have a wurtzite crystal structure and are slightly n-type doped. The GaN substrates were annealed in the open atmosphere for 10 minutes (900-1000 °C). This high-temperature treatment produced RMS values from 1- 60 nm and growth of gallium oxide (GaO) as measured with an atomic force microscopy and transmission electron microscopy respectively. A gold film (~80 nm) was deposited on the GaN surface using electron beam physical vapor deposition which was verified using ellipsometry and profilometry. The TDTR measurements suggest that the thermal conductivity decays exponentially with RMS roughness and that there is a minimum value for thermal boundary conductance at a roughness of 15nm. Future experiments will explore these results further.

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16:00 **Has ballistic heat transport by phonons been observed at room temperature?**

Authors : A. A. Maznev, K. C. Collins, J. K. Eliason, J. Cuffe, J.A. Johnson, G. Chen, K. A. Nelson
Affiliations : Dept. of Chemistry, MIT; Dept. of Mechanical Engineering, MIT; Dept. of Chemistry, MIT; Dept. of Mechanical Engineering, MIT; Paul Scherrer Institut; Dept. of Mechanical Engineering, MIT; Dept. of Chemistry, MIT

Resume : In recent years, a number of groups reported non-diffusive thermal transport at room temperature (RT). Do these observations indicate a transition to the ballistic regime with most heat carried by phonons not undergoing scattering? While at liquid He temperatures ballistic transport has been observed directly, by detecting the arrival of a heat pulse propagating at the speed of sound, the effect observed at RT is seen in the reduction of thermal conductivity compared to predictions of the Fourier law. In this report, we discuss an experiment in which the relaxation of a spatially sinusoidal thermal grating is observed using a non-contact optical technique. The simplicity of the transient grating geometry makes it amenable to theoretical analysis with the Boltzmann transport equation. Based on this analysis, we show that although low-frequency phonons with MFP>1 micrometer contribute as much as ~50% to the bulk thermal conductivity of Si at RT, their contribution to the grating relaxation is progressively reduced as the thermal grating period gets shorter. Phonons with MFP smaller than the heat transfer distance continue to dominate the heat transport until that distance is reduced to well below 100 nm. We conclude that even large deviations from the Fourier law do not, by themselves, indicate a predominantly ballistic nature of the thermal transport. A direct observation of ballistic phonon transport at temperatures >80K is still a challenge lying ahead.

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16:00 **Discrete breathers in graphene and related 2-D materials**

Authors : A. Fraile1, G. Tsironis1, N. Lazaridis1, K. Papagelis2 and D. Campbell3
Affiliations : 1) CCQCN, Department of Physics, University of Crete, Heraklion, Greece 2) Department of Materials Science, University of Patras, Greece 3) Physics Department, Boston University, MA, USA.

Resume : Discrete breathers or intrinsic localized modes have been theoretically predicted in many different materials. This is the case also of graphene [1, 2], hydrogenated graphene [3] etc. However, the results presented in [1] and [2] are not completely compatible and clearly further research is necessary. More important, experimental evidence is still lacking. In this work we present our current research using classical molecular dynamics (MD) and different interatomic potentials (Tersoff, AIREBO, LCBOP and reaxFF). Our MD simulations show the existence of breathers but, for example, the lifetime can change one order of magnitude or more depending on the force field used to describe the carbon-carbon interaction. (In fact this can be also observed comparing the lifetimes and frequencies presented in [1] and [2]). Hence, the properties of the breathers clearly depend on the interatomic potential and the differences between the potentials has to be considered. Finally we present our future experimental plans to complement our theoretical effort. References: [1] Y. Yamayose et al. Excitation of intrinsic localized modes in a graphene sheet. EPL, 80 (2007) 40008 [2] L. Z. Khadeeva et al. Discrete Breathers in Deformed Graphene. JETP Letters, 2011, Vol. 94, No. 7, pp. 539–543 [3] B. Liu et al 2013 J. Phys. D: Appl. Phys. 46 305302. Discrete breathers in hydrogenated graphene.

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16:00 **Generation of coherent pulses of 246 GHz longitudinal acoustic phonons in nipi silicon doping superlattices**

Authors : Thomas E. Wilson(a)*, Erich Kasper(b), Michael Oehme(b), Jörg Schulze(b), Konstantin Korolev(a)
Affiliations : (a) Department of Physics, Marshall University, Huntington, WV, U.S.A., 25755 (b) IHT, University of Stuttgart, Stuttgart, Germany, 70569

Resume : We report upon a novel means of producing coherent acoustic phonons; namely, the direct excitation of high-frequency acoustic phonons in silicon doping superlattices by the resonant absorption of nanosecond-pulsed far -infrared (FIR) laser radiation of the same frequency. We have used silicon-doping superlattices, fabricated on 0.6 mm thick, float zone (100) silicon substrates, with 30 periods (34.5 nm) and 2-D doping (Sb and B) concentrations of 8 x 1012 cm-2. The corresponding conversion efficiency (FIR to acoustic power) is of order 10-9. Our cavity-dumped, optically-pumped molecular FIR gas laser can provide 10-kW of peak power in 5-ns pulses at 10 pps. The FIR laser radiation is transported to the cryostat entrance window by a corrugated waveguide terminated with Teflon lens to focus the beam onto a germanium prism in contact with the superlattice. The prism coupler, operating in a total internal reflection mode, converts the incident transverse FIR electric field into an evanescent longitudinal field over the thickness of the superlattice. A fast granular aluminum/palladium current-biased microbolometer (10 micron x 20 micron x 100 nm), fabricated upon the rear sample surface and biased near its transition temperature at 1.86 K, is used for detection. Measured time-of-flight across the thin (0.6-mm) substrate is used to verify that the phonons are longitudinal. We note we observe no larger and delayed transverse acoustic phonon pulse (expected to occur with heat pulse production and phonon focusing in the (100) direction in Si), indicating that this technique provides for single-mode coherent phonon generation.

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Phonons and fluctuations in low dimensional structures

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	Phononic Crystals : Pascal Ruello (U Le Mans)	
09:00	**Hypersonic Phononic Soft Composite Materials** **Authors :** George Fytas **Affiliations :** Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany and Department of Materials Science, University of Crete and IESL-FORTH, 71110 Heraklion, Greece **Resume :** Phononic crystals, the acoustic equivalents of the photonic crystals, are controlled by a larger number of material parameters1,2. The study of hypersonic phononic crystals (hPnC) imposes substantial demand on fabrication and characterization techniques. Colloid and polymer science offer methods to create novel materials that possess periodic variations of density and elastic properties at mesoscopic length scales commensurate with the wave length of hypersonic phonons and hence photons of the visible light. The key quantity is the dispersion ω(k) of high frequency (GHz) acoustic excitations with wave vector k which is measured by the noninvasive high resolution spontaneous Brillouin light scattering. Here, examples from fabricated structures that allow manipulation of phonon propagation will be highlighted. In periodic structures of colloid based 3D-hPnC, ω(k) has revealed hypersonic phononic band gaps of different nature: Bragg gap for propagation near the edge of the first Brillouin zone due to destructive interference and hybridization gap due to the interaction of particle eigenmodes with the effective medium acoustic branch. Due to the vector nature of elastic wave propagation, 1D-hPnC (alternating layers of porous silica and PMMA) constitute model systems for fundamental studies allowing a full description of the ω(k). Under normal and oblique incidence the direction - dependent longitudinal and shear moduli are obtained at nanoscale, while the incorporation of defects (cavity and surface layers) holds a wealth of opportunities to engineer ω(k). Elastic wave propagation through hierarchically nanostructured matter can involve unprecedented mechanisms as observed in the dispersion diagram of the spider dragline silk. add to my program (close full abstract)	D.4 1
09:30	**Elastic field scattered by a resonator in an acoustic metamaterial** **Authors :** B. Bonello1, R. Marchal1, R. Moiseyenko2, Y. Pennec2, B. Djafari-Rouhani2, J. Zhao1, O. Boyko1 **Affiliations :** 1 Université Pierre et Marie Curie - Institut des NanoSciences de Paris (UMR 7588), 4 place Jussieu boîte 840 75252 Paris cedex 05 2 Institut d'Electronique, de Micro-électronique et de Nanotechnologie (IEMN–UMR CNRS 8520) Université Lille1, UFR de Physique, Cité Scientifique, 59652 Villeneuve d'Ascq Cedex, France **Resume :** Locally resonant sonic materials are artificially structured composites designed to exhibit negative effective mass density and/or elastic constants at frequencies below the Bragg band gap, giving rise to one or several forbidden bands in a frequency range where the elastic wavelength is much larger than a characteristic dimension of the resonator. In this work, we have investigated the propagation of Lamb waves in structures made either of an isolated resonant pillar or of a periodical array of resonant pillars deposited on a thin plate. The resonators and the plate are made of silicon and are designed to vibrate in the MHz range. These structures deserve special attention since pillars exhibit compressional resonant mode (monopolar) and bending resonant mode (dipolar) that may cause respectively negative modulus and negative mass density. We used a finite element method to calculate the frequencies and polarizations of	D.4 2

the normal modes of the structure, as well as the scattering of an incident Lamb wave by the pillars. These computations are then compared to experimental data recorded using a laser ultrasonic technique that maps both the phase and the amplitude of the normal displacements at the surface of the sample, resulting from the propagation of the scattered wave. At low frequency, where homogenization theory applies, the pillars vibrate in quadrature with the exciting Lamb waves when they are excited at the frequency of their compressional resonance modes. If the frequency slightly departs from the resonance, the pillars vibrate out-of-phase with respect to the incident waves. This work is supported by the Agence Nationale de la Recherche and Direction Générale de l'Armement under the project Metactif, grant ANR-11-ASTR-015.

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09:45 **Bandgap properties and directional propagations of elastic waves in two-dimensional phononic crystals with rotated cross holes** D.4 3

Authors : Yan-Feng Wang, Yue-Sheng Wang, Chuanzeng Zhang
Affiliations : Institute of Engineering Mechanics, Beijing Jiaotong University, Beijing 100044, China & Department of Civil Engineering, University of Siegen, Siegen 57068, Germany

Resume : Great efforts have been exerted in the study of wave propagation in phononic crystals, an artificial structure with periodic varying elastic properties and mass densities. Particular interests are focused on the unique characteristic of phononic crystals, i.e., the bandgap, within which the propagation of elastic waves is forbidden. Much work is devoted to the study of phononic crystals with periodic holes, the bandgaps of which are mainly determined by the geometry parameters. For the square lattice, complete bandgaps appear generally when the porosities are smaller than 0.78. Besides, complete bandgaps are also found for the grid-like structure with extremely high porosity. In spite of the bandgap properties, directional propagation of the flexural wave was numerically studied for these structures. In this paper, we will study the directional and bandgap properties of phononic crystals with rotated cross holes. The porosity of the system is relatively high. Numerical simulations are implemented by using the finite element method. The effects of the geometry parameters on the bandgaps are discussed. The vibration modes at the bandgap edges are calculated to analyze the mechanism of the bandgap generation. The contour lines of some typical bands are calculated to show the directional properties of the structure. The displacement fields of the transient response of a finite structure to a harmonic loading are also presented.

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10:00 Coffee break

10:30 **Coherent thermal phonons in Si-Ge nanoscale phononic crystals** D.4 4

Authors : N. Swinteck, K. Muralidharan, P. A. Deymier
Affiliations : University of Arizona; University of Arizona; University of Arizona

Resume : Molecular dynamics (MD) simulations are utilized to examine thermal -phonon properties in a nano-scale phononic crystal (PC) constituted of a square lattice of germanium (Ge) pillars in a matrix of silicon (Si). The Ge pillars have square cross-section and are arranged with a PC lattice constant equal to 2.715 nm. Employing Green-Kubo (GK) formalism in conjunction with spectral energy density (SED) analysis, we characterized thermal-phonon life-times in the PC from the heat-current autocorrelation function (HCAF) at 300 K. Non-decaying oscillations in the HCAF persisted for time-periods much larger than previously reported phonon life-times in bulk samples of Si or Ge at this temperature. This result indicates the existence of nearly coherent phonon modes in the PC with enhanced lifetimes. Using nonlinear phonon band structures as obtained from SED, correlations between HCAF oscillations and eigenmodes at the Gamma-point (k = 0) are obtained, signifying that band-folding effects, a consequence of phononic structural periodicity, play a leading role in ensuring coherence of thermal phonons in the Si-Ge nano-PC.

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10:45 **Transmission and attenuation of Lamb waves through a periodic array of rectangular slits in a plate** D.4 5

Authors : Rayisa P. Moiseyenko 1, Yan Pennec 1, Rémi Marchal 2, Bernard Bonello 2 and B. Djafari-Rouhani 1
Affiliations : 1 Institut d'Electronique, de Micro-électronique et de Nanotechnologie (IEMN–UMR CNRS 8520) Université Lille1, UFR de Physique, Cité Scientifique, 59652 Villeneuve d'Ascq Cedex, France; 2 Institut des NanoSciences de Paris (INSP–UMR CNRS

7588) Université Pierre et Marie Curie (box 840) 4, place Jussieu 75252 Paris Cedex 05, France
Resume : Acoustic wave transmission through sub-wavelength slits or holes, then on layers of periodically spaced cylinders and double fishnet structures, known as acoustic metamaterials has been studied in many works in relation with physical phenomena such as extraordinary resonant transmission, sound shielding etc. We present for the first time the study of analogous phenomena for Lamb waves propagating in a thin plate, in which symmetric plate mode S0 is considered. Rectangular holes are chosen due to the fact that more geometrical parameters can be varied comparatively to circular holes. In the aforementioned works the propagation medium is in general made of a fluid while the case of a solid host has been less considered. We have investigated rectangular air holes in a silicon plate and optimized the geometrical parameters in order to get a low frequency broad band attenuation. We show that, when a second row of slits is added, the choice of the distance between both rows allows for the realization of a broadband attenuation in the transmission up to 99%. With additional rows of slits we find the properties of a phononic crystal constituted by a periodic array of holes in a plate. These investigations should have implications for sound isolation and sensing applications. The work is supported by the Agence Nationale de la Recherche and Direction Générale de l'Armement under the project Metactif, grant ANR-11-ASTR-015.

11:00 **Transmission of acoustic phonons in asymmetric phononic crystals and impact on heat conduction**

Authors : T. T. Trang NGHIEM, Pierre-Olivier CHAPUIS
Affiliations : The Center for Thermal Sciences of Lyon CETHIL UMR 5008, Bât. Sadi Carnot, 9 rue de la Physique, INSA de Lyon, 69621 Villeurbanne cedex
Resume : Phononic crystals have been shown to have interesting physical properties that allow controlling sound and heat, which can both be described by the propagation of vibrations. The modification of thermal properties requires precise nanostructuration and the detailed analysis of the impact on the mean free paths. Based on results in acoustics and electronics, there have been proposals to create thermal devices such as diodes (rectifiers) or transistors. We analyze phononic crystals based on triangular holes and simulate phonon transmission experiments by solving the continuum acoustic equation in the linear elasticity case. The filtering effect usually used to rectify acoustic waves propagating in one direction is not anymore useful when considering thermal excitation which happens in all directions. As a consequence, we excite not only the acoustic waves that are perpendicular to the periodic direction, but also oblique waves. We verify that the transmission through this structure satisfies the conditions of reciprocity. The energy transmission rate can be calculated by using the spatio-temporal Fourier transforms of the acoustic Poynting vector. It is known that creating a thermal diode is only possible using non-linear systems. This work is a first step towards the implementation of non-linear equations and calculating the thermal rectification in these structures.

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Thermal Rectification : Giuliano Benenti (U Insubria)

11:15 **Heat flow asymmetries in Si-based nanostructured samples**

Authors : P. Ferrando, A. F.Lopeandia, X. Alvarez, G. Garcia, LL. Abad, M. I. Alonso, M. Garriga, A. R. Goni, J. Rodríguez-Viejo
Affiliations : Nanoamterials and Microsystems group. Dep. Physics. Universitat Autónoma de Barcelona, 08193 Bellaterra, Spain Institut de Microelectrònica de Barcelona- Centre Nacional de Microelectrónica, Campus UAB, 08193 Bellaterra, Spain. Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain
Resume : The experimental discovery of thermal rectification in asymmetrically mass-loaded carbon nanotubes in 2006 boosted the search for thermal analogs of electronic devices. However, the realization of efficient thermal rectifiers based on simple materials, such as Si or SiGe, remains a challenge. In this work, we provide experimental evidence of outstanding heat flow asymmetries in two remarkably different systems: trapezoidal Si nanowires and compositionally graded SiGe superlattices. The structure of the trapezoidal nanowires is asymmetrically defined between suspended heater/sensors by Focus Ion Beam. The origin of the heat flow asymmetry is related to the presence of Ga ions at the outer shell of the nanowire that produces a mass–damping of the oscillations with a strong influence in the atoms located at the

D.5 1

narrow outer edge of the structure. On the other hand, specific Si1-xGex/Si SLs superlattices with well-defined compositional gradients across the SiGe layer show a strong reduction of the cross plane thermal conductivity and an outstanding difference of around 40% in its value depending if the heat flow is parallel or antiparallel to the concentration gradient.

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11:45 **Theoretical thermal rectification in Si and Ge thin films**

Authors : E. Chávez-Ángel, F. Alzina, C. M. Sotomayor Torres
Affiliations : Institut Catala de Nanociencia i Nanotecnologia, ICN2,Campus UAB, 08193 Bellaterra (Barcelona), Spain Dept. of Physics, Universitat Autònoma de Barcelona, 08193 Bellaterra (Barcelona), Spain; Institut Catala de Nanociencia i Nanotecnologia, ICN2,Campus UAB, 08193 Bellaterra (Barcelona), Spain; Institut Catala de Nanociencia i Nanotecnologia, ICN2,Campus UAB, 08193 Bellaterra (Barcelona), Spain Institucio Catalana de Recerca i Estudis Avançats, ICREA, 08010 Barcelona, Spain

Resume : A deep understanding of heat transport in low-dimensional semiconductor structures is a topic of increasing research activities driven by the need for a more energy conscious society. This is motivated, in part, by the increasing importance of thermal management as a consequence of the large power densities resulting from the continuous miniaturization of electronics components. In this sense, the thermal rectification at nano/microscale is attracting an increasing scientific attention due to its promising potential for thermal management and energy efficiency. Moreover, in analogy with the electrical diode, the thermal rectifier or diode becomes an essential building block of thermal logic circuits. In the present work, the different temperature dependence of the thermal conductivity between two materials is studied for thermal rectification. Four different combinations of silicon and germanium films had been studying. Thermal conductivities are calculated using Fuchs-Sondheimer boundary corrections. The theoretical predictions suggest values of 0.5 to 10 % of efficiency in Si-Si and 0.4 to 12 % in Si-Ge systems

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12:00 **Heat transport across a SiGe nanowire axial junction: interface thermal resistance and thermal rectification**

Authors : R. Rurali (1), X. Cartoixe (2), L. Colombo (3)
Affiliations : (1) Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC), Spain (2) Universitat Autonoma de Barcelona, Spain (3) Universita di Cagliari, Italy

Resume : Semiconducting nanowires (NWs) have attracted a growing interest in recent years and are recognized as important building blocks for emerging applications in nanoelectronics [1-3]. The understanding of thermal transport has lately acquired a great importance as well, because NWs have been proposed to be a pathway for the engineering of efficient thermoelectric materials. Here we study thermal transport in SiGe nanowires across a Si/Ge axial interface by means of non-equilibrium molecular dynamics simulations. We calculate the interface thermal resistance (ITR) of realistic models of axial SiGe heterojunctions, whose morphology depends strongly on the different experimental conditions [4-7]. We also investigate if these asymmetric junctions can yield thermal resistances that depend on the applied thermal gradient, i.e. thermal rectification. We find that diffuse interfaces result in larger ITR, while sharp junctions yield a small, but non-negligible thermal rectification, favoring heat transport from Si to Ge. [1] D. K. Ferry, Science 319, 579 (2008) [2] R. Rurali, Rev. Mod. Phys. 82, 427 (2010) [3] M. Amato, M. Palummo, R. Rurali, and S. Ossicini, Chem. Rev., doi:10.1021/cr400261y [4] Clark et al., Nano Lett. 8, 1246 (2008) [5] Wen et al., Science 326, 1247 (2009) [6] Perea et al., Nano Lett. 11, 3117 (2011) [7] Geaney et al., Nano Lett. 13, 1675 (2013)

D.5 3

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12:15 **Photonics for Radiative Thermal Rectification**

Authors : Elyes Nefzaoui, Jérémie Drevillon, Younès Ezzahri, Karl Joulain
Affiliations : Institut Pprime (CNRS) - Université de Poitiers - ENSMA / CETHIL (CNRS) - INSA Lyon, Institut Pprime (CNRS) - Université de Poitiers - ENSMA, Institut Pprime (CNRS) - Université de Poitiers - ENSMA, Institut Pprime (CNRS) - Université de Poitiers - ENSMA

Resume : Thermal rectification can be defined as an asymmetry in the heat flux when the temperature difference between two interacting thermal reservoirs is reversed. A non-zero rectification means that a reversal of the thermal gradient induces, in addition to the reversal of the heat flux direction, a variation of its magnitude. The realization of a device exhibiting such an "uncommon" behavior, a thermal rectifier for instance, would pave the way to the development of thermal circuits in the manner non-linear electronic devices marked the genesis of modern electronics. Consequently, an increasing interest has been given to

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thermal rectifiers during recent years. Until the end of the last decade, all proposed rectifiers managed heat transport in solids. Very recently, the first photon mediated rectification devices have been proposed, exclusively based on near-field radiative transfer between bulk materials. In the present contribution, we first draw up a map of previously proposed radiative thermal rectifiers on the basis of an unequivocal definition of the rectification ratio and through an extensive review of photon mediated thermal rectification literature. Then, we present the first model of a tunable far-field radiative thermal rectifier based on particular photonic structures and illustrate it with different implementations.

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12:30 **Lunch break**

Coherent Acoustic Phonons and Phonon Sources : Thomas Dekorsy (U Konstanz)

14:00 **Coherent Acoustic Phonons and Phonon Sources**

Authors : Bernard Perrin, Romain Legrand, Agnès Huynh
Affiliations : Institut des NanoSciences de Paris, UMR 7588 CNRS - Université Pierre & Marie Curie 140 Rue de Lourmel, 75015 Paris – Fr

Resume : The association of MBE techniques, to obtain high quality semiconducting heterostructures, and of pump-probe methods, which allow achieving a very high temporal resolution, gives now the opportunity to realize terahertz coherent acoustics experiments [1-6]. We will first explain how semiconducting superlattices can be used as excellent coherent phonons emitters and detectors in the subterahertz to terahertz range and then describe a few configurations to study coherent phonons propagation on macroscopic distances. Finally we will show how these experiments can be used to determine longitudinal phonons mean free path over a large frequency range (0.2 – 1 THz) and a temperature domain ranging from 4 K to 60-80K. These data will be compared to theoretical calculations. 1) P. Hawker, A. J. Kent, L. J. Challis, A. Bartels, T. Dekorsy, H. Kurtz, K. Khöler, Appl. Phys. Lett. 77, 3209 (2000) 2) Cheng-Ying Chen, Yu-Chieh Wen, Hung-Ping Chen, Tzu-Ming Liu, Chang-Chi Pan, Jen-Inn Chyi and Chi-Kuang Sun, Appl. Phys. Lett. 91, 133101 (2007) 3) M. Trigo, T. A. Eckhause, J. K. Wahlstrand, R. Merlin, M. Reason, R. S. Goldman, R. S., Appl. Phys. Lett. 91, 023115 (2007) 4) A. Huynh, B. Perrin, N. Lanzillotti-Kimura, B. Jusserand, A. Fainstein and A. Lemaître, Phys. Rev. B 78, 233302 (2008) 5) A Huynh, B. Perrin, B. Jusserand, A. Lemaître, Appl. Phys. Lett. 99, 191908 (2011) 6) M. F. Pascual-Winter, A. Fainstein, B. Jusserand, B. Perrin, A. Lemaître , Phys. Rev. B85, 235443 (2012)

D.6 1

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14:30 **Coherent acoustic phonons emission driven by hot electrons**

Authors : M. Lejman, V. Shalagatskyi, O. Kovalenko, T. Pezeril, V. Temnov, P. Ruello
Affiliations : Institut des Molécules et Matériaux du Mans, UMR 6283 CNRS, Université du Maine

Resume : The understanding of the transport of hot electrons and their interactions with the bulk lattice and the interface is of prime importance for the improvement of advanced nanoscale devices. In this communication, we show that supersonic hot electrons are responsible for the emission of coherent acoustic phonons deeply beneath the free surface where they are optically excited consistently with previous experiments [1-3]. Moreover, these hot electrons can also travel enough far at room temperature to interact with a buried interface (Cu-Ti in our case) located at 220 nm beneath the free surface. In particular, we evidence that this interaction leads to coherent acoustic phonon emission. Such phenomenon has been reported only one time up to now in the case of aluminum [4]. In order to go deeper in the experimental investigations and to discuss in more details the underlying physics, several ultrafast optical pump-probe configurations been used [2]. In particular, we have performed different experiments where the time of flight of hot electrons and coherent acoustic phonons have been characterized. From an original probe wavelength dependence study of the optical detection process, we clearly establish the signature of superdiffusive hot transport within the copper film and the link with the acoustic phonon emission. These results and observations are important to quantify the mechanism of electron-phonon interaction at materials interfaces. [1] O. B. Wright, "Ultrafast nonequilibrium stress generation in gold and silver," Phys. Rev. B 49, 9985–9988 (1994). [2] O. B. Wright and V. Gusev, "Ultrafast generation of acoustic waves in copper," IEEE Trans. Ultrason.

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Ferroelectr. Freq. Control 42, 331–338 (1995). [3] G. Tas and H. J. Maris, "Electron diffusion in metals studied by picosecond ultrasonics," Phys. Rev. B 49, 15046–15054 (1994). [4] M. Lejman, V. Shalagatskyi, O. Kovalenko, T. Pezeril, V. Temnov, P. Ruello "Ultrafast optical detection of coherent acoustic phonons emission driven by superdiffusive hot electrons", J. Opt. Soc. Am. B, to be published in Feb 2014.

14:45 **Boundary Limited Thermal Conductivity of Crystalline Rods Oriented near Phonon Focusing Caustics**

Authors : A.G. Every1 , A.A. Maznev2
Affiliations : 1School of Physics, University of the Witwatersrand, PO Wits 2050, Johannesburg, South Africa 2Department of Chemistry, Massachusetts Institute of Technology, Cambridge MA 02139, USA

Resume : In specimens of sufficiently small size and/or at sufficiently low temperature, surface scattering of phonons dominates over bulk scattering. In the Casimir model [1] for boundary limited thermal conduction in a long rod, phonon scattering at the surfaces is assumed to be perfectly diffuse. This model yields a formula for the overall phonon mean free path that is an average over all phonon modes, with a weighting factor proportional to cos(t)^2/sin(t), [2] where t is the angle between the mode group velocity and the rod axis. It follows that phonons with velocities close to the rod axis provide a large contribution to the heat transport. Elastic anisotropy has a pronounced affect on the ballistic transport of thermal phonons, with the phonon flux for a particular branch in any direction being proportional to the Maris phonon enhancement factor,[3] which in turn is inversely proportional to the local Gaussian curvature of the acoustic slowness surface. Striking patterns of phonon caustics are observed in phonon imaging experiments,[4] that correspond to directions of vanishing Gaussian curvature and infinite phonon enhancement. A tendency has been noted [2] for the Casimir conductivity to be higher in focusing directions, but a clear analytical relationship between the two not before now established. The question we address in this paper is what happens if the rod axis points exactly in the direction of a phonon focusing caustic, or deviates slightly from the caustic direction. Three cases of the singular behavior near structurally stable caustics are considered (a) rod axis directions near a line caustic associated with a fold in the acoustic wave surface, (b) rod axis directions near a cusp caustic, along and perpendicular to the direction the cusp is pointing, and (c) rod axis directions near an external conical refraction caustic, a highly degenerate caustic that exists for certain hexagonal (transversely isotropic) crystals. We show that the thermal conductivity of an infinite rod oriented along the external conical refraction caustic formally diverges, whilst in the cases of the fold and cusp caustics, the conductivity remains finite. Numerical results are presented for zinc, with the slow transverse branch providing examples of the external conical refraction and fold caustics. [1] H. B. G. Casimir, Physica 5, 495 (1938). [2] A. K. McCurdy, H. J. Maris, and C. Elbaum, Phys. Rev. B2, 4077 (1970); A. K. McCurdy, Phys. Rev. B9, 466 (1974). [3] H. J. Maris, J. Acoust. Soc. Am. 50, 812 (1971). [4] J.P. Wolfe, Imaging Phonons, Cambridge University Press, Cambridge, 1998.

D.6 3

15:00 **Measurement of coherent single-pass amplification of sub-Terahertz phonons**

Authors : C L Poyser, A V Akimov, R P Campion, A J Kent
Affiliations : School of Physics and Astronomy, University of Nottingham, University Park, Nottingham NG7 2RD UK

Resume : We describe the use of an AlGaAs p-i-n diode to monitor the output of a single pass phonon amplification device. The optical resonance of quantum wells, incorporated in the intrinsic region of the diode, strongly depend on the strain associated with acoustic waves. This can be exploited to create an optically-gated detector with picosecond resolution by monitoring changes in induced photocurrent caused by acoustic waves [1]. In the current scheme, the p-i-n detector is fabricated on one side of a 150μm GaAs substrate, and two GaAs/AlAs superlattices (SLs), the lower of which can be placed under an electrical bias, are grown on the other side. The lower, SASER gain, SL was grown to specifications which have been previously shown, using an incoherent bolometric detection technique, to provide phonon amplification [2]. Femtosecond optical pumping of the top SL generates quasi-monochromatic sub -Terahertz phonons which propagate through the gain SL and the substrate to the p-i-n diode. This is gated by a time-delayed femtosecond pulse providing a high resolution coherent detection, this shows evidence of coherent amplification

D.6 4

in the SASER device. [1] Moss, D et al. Phys. Rev. B 83, 245303 (2011) [2] Beardsley, R. P. et al. New J. Phys. 13, 073007 (2011)

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15:15 **Modeling of high-frequency electromechanical instability of graphene nano-ribbons** D.6 5

Authors : M.Eriksson, L.Gorelik, M.Voinova

Affiliations : Chalmers University of Technology, Goteborg, Sweden

Resume : Rapid progress in nanomanufacturing and applications of 2D carbon materials and, in particular, of graphene-based systems, stimulated new experimental and theoretical efforts in studying the interplay between optic, electronic, and mechanical properties of these unique structures [1,2]. In the present work we have theoretically studied the mechanical vibrations of a graphene nano-ribbon in a high frequency electro-magnetic field. We considered a deflection of nano-ribbon membrane of graphene suspended over the trench between two conducting substrates. We report that despite of the external field frequency is much higher than the eigenfrequency of the graphene membrane, one can find the instability and its self-sustained mechanical oscillations with the fundamental frequency of the ribbon. Our results show the principal way of applications of electromechanical effects in graphene nano-ribbons for electro-optomechanical transduction. [1] Dafei Jin, Anshunam Kumar, Kin Hung Fung, Jun Xu, and Nicholas X.Fang. Terahertz plasmonics in ferroelectric-gated graphene. Appl. Phys. Lett. 102, 201118 (2013) [2] M. Eriksson, D. Midtvedt, A. Croy, A. Isacsson. Frequency tuning, nonlinearities and mode coupling in circular mechanical graphene resonators. http://arxiv.org/pdf/1305.3741v2.pdf

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15:30 Coffee break

Thermoelectricity and Energy Conversion in the nanoscale : George Fytas (FORTH and MPI)

16:00 **Efficient reduction of thermal conductivity in silicon using phononic-engineered membranes** D.7 1

Authors : 1,2V. Lacatena, 1,2M. Haras, 2,J.-F. Robillard, 1,S. Monfray, 1,T. Skotnicki, 2,E. Dubois

Affiliations : 1: STMicroelectronics 850, rue Jean Monnet, F-38926 Crolles FRANCE 2: IEMN UMR CNRS 8520, Institut d'Electronique, de Microélectronique et de Nanotechnologie, Avenue Poincaré, F-59652 Villeneuve d'Ascq FRANCE

Resume : Phononic crystals (PC) have been a remarkably active research field for more than two decades [1]. The principle of Bragg reflection on an artificial crystal-like structure leading to additional spectral (band gaps) and refractive (negative refraction, anisotropy) properties is scalable in any frequency range by a suitable choice of the crystal lattice constant. Recent works have demonstrated nanoscale PCs as a mean for reducing the thermal conductivity by a modulation of the thermal phonon propagation [2-4]. Such phononic engineered structures are promising candidates as efficient thermoelectric materials compatible with CMOS technology since the lattice thermal conductivity can be reduced without affecting the electrical conductivity and thus increase the thermoelectric figure of merit zT. In this work we present experimental results including: i) the fabrication of phononic crystals in 70 nm thick SOI and ii) integrated heater and sensor devices for thermal conductivity measurements. Finally, molecular dynamics simulations based on Green Kubo method will be presented [5]. [1] M.S. Kushwaha et al, Phys. Rev. Lett. 71, 2022 (1993) [2] J.-K. Yu et al, Nat. Nanotechnol., 5, 718 (2010) [3] P. E. Hopkins et al, Nano Lett., 11, 107 (2011) [4] J. Tang et al, Nano Lett, 10, 4279 (2010) [5] S. G. Volz et al, Phys. Rev. B, 61, 2651, (2000)

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16:30 **Characterization of a thin film Si-based planar u-TEG** D.7 2

Authors : A.F. Lopeandía#; A.P. Perez-Marín#; Ll. Abad&; P. Ferrando#; G. Garcia#; J.Rodríguez-Viejo#;

Affiliations : #Grupo de Nanomateriales y Microsistemas, Dep. Física, Universitat Autónoma de Barcelona, 08193 Bellaterra, Spain. &Instituto de Microelectrónica de Barcelona- Centre Nacional de Microelectrónica, Campus UAB, 0893 Bellaterra, Spain.

Resume : We report the characterization of a thermoelectric microgenerator build up using standard CMOS technologies. As a thermoelectric active material we use ultrathin single-crystalline Si membranes, 100 nm in thickness, with

embedded n and p-type doped regions. The planar design, with the n-p couples electrically connected in series and thermally in parallel, includes a central heater/sensor that permits to impose several small temperature gradients and then characterize the average thermoelectric lumped parameters. Finite element modeling is used to derive, from the experimental data, the intensive parameters for the thin film couples, and thus evaluate ZT in the full range measured from 50 to 350K. A 3-fold reduction in thermal conductivity due to the phonon boundary scattering with the thin film surfaces supposes an effective improvement in ZT respect to bulk values since resistivity and Seebeck coefficients are respected. The ZT obtained grows monotonically in the measured range. As a test of the maximum output power density produced, we imposed a 200K temperature gradient with the frame at 350K obtaining 250 μW/cm^2.

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16:45 **Thermal Conductivity Suppression in Thin Silicon Nanowires and Strategies for its Reduction in Larger-Diameter Wires**

Authors : A. Cowley (1), D. Byrne (1), N. Bennett (1,2)
Affiliations : (1) Nanomaterials Processing Lab., School of Electronic Engineering, Dublin City University, Dublin 9, Ireland. (2) Institute of Mechanical, Process and Energy Engineering, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom.

Resume : It is well known that bulk silicon gives poor thermoelectric performance relative to established materials like Bismuth Telluride. However, Si nanowires represent a potentially low-cost, scalable thermoelectric material owing to their reduced thermal conductivity. Nanowires are effective at scattering long-wavelength phonon modes, which strongly contribute to the thermal transport in bulk Si, while leaving the electronic transport within the wire largely unaffected. We present a systematic experimental study into Si nanowires fabricated using metal-assisted chemical etching (MACE), and address the relationship between nanowire structure and thermal conductivity reduction. We also detail a novel, second-stage to the MACE process, whereby large-scale nanostructure feature modification can be readily achieved via a further electrochemical etch treatment utilizing Ag nanoparticles. This secondary process has the potential to increase the thermoelectric performance of larger-diameter Si nanowires. Results showing thermal conductivity variation as a function of these processing steps, in addition to TEM and SEM measurements, are presented. This study represents a potential methodology for the low-cost performance enhancement of Si nanowires for thermoelectric applications.

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17:00 **Thermoelectric Properties of New Graphene Allotropes**

Authors : Tao Ouyang and Ming Hu
Affiliations : Institute of Mineral Engineering (GHI), Division of Materials Science and Engineering, RWTH Aachen University, Mauerstrasse 5, 52064 Aachen, Germany

Resume : Thermoelectric materials have aroused widespread interest from both theoretical and technological researches due to the advantage that they can directly convert heat to electricity and vice versa. Using the Nonequilibrium Green's function method, we investigate the thermoelectric properties of new graphene allotropes. Compared with graphene, the allotrope and its nanostructures are found to possess superior thermoelectric performance. This improvement mainly originates from the weak thermal transport ability and unique electronic transport properties owning to the novel geometric structures in the new graphene allotropes. For example, the results show that the thermoelectric figure of merit (ZT) of gamma graphyne nano-ribbons is about 3 - 13 times larger than that of the graphene nano-ribbons. Meanwhile, the thermoelectric performance of this nano-materials can be further enhanced (the ZT value can even exceed 1.0 at room temperature) when width discrepancy between the left and right leads is introduced. As for the other graphene allotropes, some interesting thermal transport and thermoelectric properties have also been observed. The findings qualify the graphene allotropes as a promising candidate for thermoelectric applications and provide useful guideline for enhancing the thermoelectric performance for experimentalists.

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17:15 **Increasing thermoelectric efficiency: Dynamical models unveil microscopic mechanisms**

Authors : Giuliano Benenti
Affiliations : University of Insubria, Italy

Resume : The understanding of coupled particles and heat transport in complex systems is a fundamental problem, also of practical interest in connection with

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the challenging task of developing high-performance thermoelectric heat engines and refrigerators. Recently discovered general mechanisms of optimizing the figure of merit of thermoelectric efficiency are discussed, also in connection to momentum-conserving interacting systems [1.2], to the breaking of time-reversal symmetry by an applied magnetic field [3-6], and to multiterminal steady-state quantum thermal machines [7]. [1] G. Benenti, G. Casati and W. Jiao, Conservation laws and thermodynamic efficiencies, Phys. Rev. Lett. 110, 070604 (2013). [2] G. Benenti, G. Casati and C. Mejia-Monasterio, Thermoelectric efficiency in momentum-conserving systems, New J. Phys. 16, 015014 (2014). [3] G. Benenti, K. Saito and G. Casati, Thermodynamic bounds on efficiency for systems with broken time-reversal symmetry, Phys. Rev. Lett. 106, 230602 (2011). [4] K. Saito, G. Benenti, G. Casati and T. Prosen, Thermopower with broken time-reversal symmetry, Phys. Rev. B 84, 201306(R) (2011). [5] M. Horvat, T. Prosen, G. Benenti and G. Casati, Railway switch transport model, Phys. Rev. E 86, 052102 (2012). [6] V. Balachandran, G. Benenti and G. Casati, Efficiency of three-terminal thermoelectric transport under broken time-reversal symmetry, Phys. Rev. B 87, 165419 (2013). [7] F. Mazza, R. Bosisio, G. Benenti, V. Giovannetti, R. Fazio and F. Taddei, Thermoelectric efficiency of three-terminal quantum thermal machines, preprint.

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Phonons and fluctuations in low dimensional structures

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start at	Subject	Num.
	Optomechanics : Achim Kittel (U Oldenburg)	
09:00	**Cavity optomechanics: controlling phonons with photons at the quantum level** **Authors :** Tobias J. Kippenberg **Affiliations :** Institute of Condensed Matter Physics, EPFL Switzerland **Resume :** The mutual coupling of optical and mechanical degrees of freedom via radiation pressure has been a subject of interest in the context of quantum limited displacements measurements for Gravity Wave detection for many decades. Over the past years these radiation pressure "backaction" phenomena have been observed – starting from observations in in high Q optical microresonators(1) – in a variety of micro and nanoscale opto and electro-mechanical systems. The high Q of the microresonators, not only enhances nonlinear phenomena - such as optical frequency comb generation(2) via the Kerr nonlinearity – but also enhances the radiation pressure interaction. This has allowed the observation of radiation pressure phenomena in an experimental setting and constitute the fast developing research field of cavity quantum optomechanics(3, 4). I will describe a range of optomechanical phenomena studied using on-chip optical microresonators, that combine both optical and mechanical degrees of freedom in one and the same device. Radiation pressure back-action of photons is shown to lead to effective cooling(5 -8) of the mechanical oscillator mode using dynamical backaction. Cooling to the quantum regime is possible using sideband resolved cooling, with passive of cryogenic precooling to ca. 700 mK, which enables cooling the oscillators such that it resides in the quantum ground state more than 1/3 of its time(9). Increasing the mutual coupling further, it is possible in this regime to observe quantum coherent coupling(9) in which the mechanical and optical mode hybridize and the coupling rate exceeds the mechanical and optical decoherence rate (7). In this regime the mechanical and optical mode form an optomechanical 'polariton'. This enables a range of quantum optical experiments, including state transfer from light to mechanics using the phenomenon of optomechanically induced transparency(10). In addition experiments are described that utilized the optomechanical coupling for highly efficient force measurements using nanomechanical oscillators(11), as well as elements enabling switching, slowing or advancing of radiation(12). References: 1. T. J. Kippenberg et al., Analysis of Radiation-Pressure Induced Mechanical Oscillation of an Optical Microcavity. Physical Review Letters 95, 033901 (2005). 2. T. J. Kippenberg, R. Holzwarth, S. A. Diddams, Microresonator-based optical frequency combs. Science 332, 555 (Apr 29, 2011). 3. T. J. Kippenberg, K. J. Vahala, Cavity Optomechanics: Backaction at the mesoscale. Science 321, 1172 (2008, 2008). 4. M. Aspelmeyer, T. J. Kippenberg, F. M. Marquardt, Cavity Optomechanics. http://arxiv.org/abs/1303.0733, (2012). 5. V. B. Braginsky, S. P. Vyatchanin, Low quantum noise tranquilizer for Fabry-Perot interferometer. Physics Letters A 293, 228 (Feb 4, 2002). 6. V. B. Braginsky, Measurement of Weak Forces in Physics Experiments. (University of Chicago Press, Chicago, 1977). 7. A. Schliesser et al., Radiation pressure cooling of a micromechanical oscillator using dynamical backaction. Physical Review Letters 97, 243905 (Dec 15, 2006). 8. A. Schliesser et al., Resolved-sideband cooling of a micromechanical oscillator. Nature Physics 4, 415 (2008). 9. E. Verhagen et al., Quantum-coherent coupling of a mechanical oscillator to an optical cavity mode. Nature 482, 63 (Feb 2, 2012). 10. S. Weis et al., Optomechanically induced transparency. Science 330, 1520 (Dec 10, 2010). 11. E. Gavartin, P. Verlot, T.	D.8 1

J. Kippenberg, A hybrid on-chip optomechanical transducer for ultrasensitive force measurements. Nature nanotechnology 7, 509 (Aug, 2012). 12. X. Zhou et al., Slowing, advancing and switching of microwave signals using circuit nanoelectromechanics. Nature Physics 9, 179 (2013).

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09:30 **Investigation of optomechanical interactions in two-dimensional phoxonic crystal cross-slot cavities and hetero-structure cavities**

Authors : Tian-Xue Ma, Yue-Sheng Wang, Chuanzeng Zhang
Affiliations : Institute of Engineering Mechanics, Beijing Jiaotong University, Beijing 100044, PR China; Institute of Engineering Mechanics, Beijing Jiaotong University, Beijing 100044, PR China; Department of Civil Engineering, University of Siegen, Siegen, D-57068, Germany

Resume : In recent years, periodic structures with simultaneous photonic and phononic bandgaps are of interest for the potential applications to new acousto-optical devices and the enhancements of optomechanical or acousto-optical interactions. These structures which can control and localize both light and sound in the same spatial region at the same time are termed phoxonic crystals (PXCs) or optomechanical crystals. Recently, we theoretically investigated the properties of photonic and phononic bandgaps in two-dimensional (2D) silicon PXCs with veins. Large complete photonic and phononic bandgaps can be simultaneously obtained in such structures. Based on the vein-PXC in a square lattice, we design the cross-slot cavities and hetero-structure cavities. All calculations in this article are performed using the finite element method (COMSOL Multiphysics). By varying the structural parameters, both elastic and optical waves can be simultaneously localized in the cavity regions of these two kinds of cavities. Two mechanisms which contribute to the optomechanical coupling, namely the bulk photoelastic effect and the interface motion are considered in the present work. Optomechanical coupling of in-plane phononic mode with both transverse magnetic (TM) and transverse electric (TE) photonic modes are studied. We analyze the temporal modulation of the photonic mode frequency by acoustic vibrational motion during one period of the acoustic oscillations. We note that the 2D PXC cavities presented here can be references for further design of acousto-optical devices in applications for optical communication, chemical and biomedical sensing, etc.

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09:45 **Theory and simulation of optomechanical effects in phoXonic crystals**

Authors : Said El-Jallal1,2, Mourad Oudich1, Yan Pennec1, Abdelkader Makhoute2, Jordi Gomis-Bresco3, Daniel Navarro-Urrios 3, Clivia M. Sotomayor Torres3, Alejandro Martínez4, Bahram Djafari-Rouhani1
Affiliations : 1Institut d'Electronique, de Microélectronique et de Nanotechnologie, UMR CNRS 8520, Université Lille 1, Villeneuve d'Ascq, France ; 2PRILM, Université de Moulay Ismail, Faculté des sciences, Meknès, Morocco ; 3Catalan Institute of Nanotechnology, Campus UAB, 08193 Bellaterra (Barcelona), Spain; 4Nanophotonics Technology Center, Universidad Politécnica de Valencia, Spain.

Resume : Phoxonic crystals are periodic structures that can exhibit dual phononic and photonic band gaps, thus allowing the simultaneous confinement of both acoustic and optical waves inside the same defect such as a cavity or a waveguide. Then, one can expect an enhancement of the phonon-photon interaction for the purpose of novel optomechanical devices, in particular for the modulation of light by acoustic waves. We study Theoretically the optomechanic interaction in different (2D[1], slabs[2], and strips phoxonic crystals cavities. We take into account both mechanisms that contribute to the acousto-optic interaction, namely the photoelastic and moving interface effects. The strength of the acousto-optic coupling is evaluated for each phonon-photon pair by calculating either the modulation of the photonic frequency by the acoustic mode or the so-called coupling rate. The contributions of the photoelastic and moving interfaces effects can have similar or very different magnitudes. Moreover, they can be in phase and add together or be out of phase and partly cancel each other. We can notice that, due to symmetry reasons, only acoustic modes having a specific symmetry can couple to photonic modes. Finally, we discuss the influence of the material properties as concerns the photoelastic effect [1] since the latter strongly changes when the optical frequency approaches the energy of the direct band gap. [1]S Eljallal et al JPCM 26, 015005(2014) [2]S Eljallal et al PRB 88, 205410(2013)

D.8 3

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10:00 **Coffee break**

Theoretical and Computational Methods : Bahram Djafari-Rouhani (IEMN)

10:30 **Theory of interface and anharmonic phonon interactions in nanocomposite materials**

Authors : G. P. Srivastava, I. O. Thomas*
Affiliations : School of Physics, University of Exeter, Exeter EX4 4QL, UK *Present address: School of Physics, University of Durham, Durham DH1 3LE, UK

Resume : We present a theory of phonon scattering rates resulting from mass smudging across interfaces and from anharmonicity in nanocomposite materials [1]. The formalism is employed for computing the lattice thermal conductivity of thin-layer semiconductor superlattices, based on the solution of the phonon Boltzmann transport equation within the single-mode relaxation time approximation. Experimental results available for ultra-short period Si/Ge[001] superlattices are explained with the help of our numerical results. We estimate that a realistically small amount of interface mass smudging results in a reduction of around 3-14\% in the cross-plane conductivity component for the superlattice of periodicty 4.4 nm and sample size 4.4 mm in the temperature range 100-700 K when boundary scattering is relatively weak. We further estimate that the cross-planar thermal conductivity is roughly 4.1-4.8 times smaller than the in-plane thermal conductivity components. [1] I. O. Thomas and G. P. Srivastava, Phys. Rev. B 88, 115207 (2013).

D.9 1

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11:00 **Cross-mode correlations, localized modes, and heat conduction in anharmonic oscillator chains**

Authors : Maxime Gill-Comeau, Laurent J. Lewis
Affiliations : Département de physique, Université de Montréal

Resume : We study current-current fluctuations in anharmonic oscillator chains which are related to heat conductivity by a Green-Kubo relation. For low anharmonicity levels, we observe significant cross-mode correlations in contradiction with the independent mode hypothesis generally used to motivate relaxation-time models. We find that these correlations are important as they seem to inhibit relaxation and are associated with different scaling laws for conductivity as a function of anharmonicity. However, these correlations do not seem to be crucial for anomalous conduction as they are present also in regular models. The correlation patterns seem to indicate that they are associated with localized modes, indicating that these modes might be the main heat carriers in the low anharmonicity regime. Also, the decay rate of the cross-mode correlations and the largest Lyapunov exponent of the system were found to follow similar scaling laws, suggesting that the two properties are linked.

D.9 2

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11:15 **Phonons at amorphous/crystalline silicon interfaces**

Authors : Konstantinos TERMENTZIDIS 1, Arthur FRANCE-LANORD 1, Etienne BLANDRE 1, Samy MERABIA 2, Tristan ALBARET 2 and David LACROIX 1
Affiliations : 1 LEMTA, CNRS UMR-7563, University of Lorraine, Vondoeuvre les Nancy, France 2 ILM, CNRS, University of Lyon 1, Lyon, France

Resume : Silicon is considered as a reference material both for its crystalline and amorphous phases. While each phase separately has been investigated extensively, less attention is given to nanostructures involving both phases and especially their interfaces. Yet, almost all silicon devices contain such interfaces and the transport for both electrons and phonons through them is a crucial issue. In this study, we model amorphous/crystalline interfaces for nanowires and superlattices. The aim is to predict the thermal properties of these nanostructured materials, and explain the trends with the phonon density of states and the Kapitza resistance. The calculations have been done with molecular dynamics method, using a realistic interatomic potential. The thermal conductivity of both nanostructures is found to be close to the bulk amorphous one and almost independent the temperature. In bulk amorphous silicon, the vibrational features of the crystalline phase are present but smoothed out, due to the lack of periodicity. The localized modes and the large depression of the high frequency phonons, which have been proved to carry heat even if they are nonpropagating diffusive modes, contribute to the reduction of the thermal conductivity. We will present also the local phonon density of states at different

D.9 3

locations on both sides of a planar interface. The phonons feel the interfaces in a distance of roughly 4Å away from them.

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11:30 **Approach-to-equilibrium molecular dynamics for thermal conductivies and boundary conductances**

Authors : P. L. Palla, E. Lampin, P.-A. Francioso and F. Cleri
Affiliations : IEMN UMR CNRS 8520 and University of Lille - CS 60069 - 59625 Villeneuve d'Ascq Cedex- France

Resume : Thermal transport is simulated at the atomic scale by approach-to-equilibrium molecular dynamics simulations (AEMD) [1]. In this method, a hot and a cold regions are delimited, before the approach-to-equilibrium is simulated by releasing the thermal constraint. The temperature difference between the two regions is monitored during the approach-to-equilibrium. It proceeds by an exponential decay. The decay time is used to extract thermal properties of the system. In the case of a bulk material, the conductivity is determined thanks to the comparison with the heat equation solution. The extrapolated value for silicon modeled by Tersoff potential [2] is compared to other calculations and an excellent agreement with previous calculations [3] is obtained. AEMD is also applied to interfaces and nanoconstrictions. In these cases the decay time of the temperature difference is related to boundary conductances. The application is made for interfaces between good conductors but also for less favorable cases of interfaces between a good and a poor conductor. Even in this last configuration, the approach is shown to be sensitive enough to extract the conductance [4]. [1] E. Lampin, P. L. Palla, P.-A-Francioso and F. Cleri, J. Appl. Phys. 114, 033525 (2013) [2] J. Tersoff, Phys. Rev. B 38, 9902 (1988) [3] P. C. Howell, J. Chem. Phys. 137, 224111 (2012) [4] E. Lampin et al, Appl. Phys. Lett. 100, 131906 (2012)

D.9 4

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11:45 **Boundary scattering of phonons: what is the specularity of a randomly rough surface?**

Authors : A. A. Maznev
Affiliations : Dept. of Chemistry, MIT

Resume : Boundary scattering of phonons has a profound effect on thermal transport in nanostructures. The model of perfectly diffuse scattering proposed by Casimir is widely used to analyze thermal conductivity in thin films and nanowires. However, surfaces tend to become specular for long wavelengths or at grazing incidence angles, and the specularity parameter is often invoked to explain discrepancies between the diffuse scattering model and the experimental data. Despite extensive literature on wave scattering from rough surfaces, a comprehensive analysis of phonon scattering by a randomly rough surface appears to be still lacking. Researches typically rely on a simple analytical equation, often ascribed to Ziman, that relates specularity to roughness. In this report, we will show that Ziman's equation is only valid in Kirchhoff's approximation that assumes the correlation length of surface roughness to be much greater than the acoustic wavelength. Furthermore, we will present a perturbation analysis of acoustic wave scattering by a randomly rough boundary of an elastic half-space that accounts for scattering into bulk transverse and longitudinal waves as well as into Rayleigh surface waves. We will present numerical calculations for normally incident longitudinal and transverse waves along with analytical expressions for limiting cases and discuss the implications of the results in view of recent experiments on thermal transport and sub-THz coherent phonons in thin Si membranes.

D.9 5

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12:00 **Numerical calculation of optical phonon decay rate in InN/GaN MQW and its bulk counterparts**

Authors : Hongze Xia, Rob Patterson, Yu Feng, Tran Smyth, Yuanxun Liao, Pengfei Zhang, Xi Dai, Neeti Gupta, Xiaoming Wen, Simon Chung, Xuguang Jia, Lingfeng Wu, Binesh Puthen-Veettil, Shujuan Huang, Santosh Shrestha, Gavin Conibeer
Affiliations : The University of New South Wales

Resume : Anharmonic decay of high frequency phonons into low frequency vibrations is a significant energy loss mechanism in semiconductors. In the field of Hot Carrier Solar Cells (HCSC), preventing this decay is of great importance as it helps increase hot carriers lifetime. It also has major impact in quantum information processing, where this kind of anharmonicity could lead to decoherence in quantum information transfer. Phonon decay in nano-crystals like quantum dots and multiple quantum wells (MQWs) has not been extensively studied in the literature. In this work, the anharmonic decay of longitudinal optical (LO) phonons in an InN/GaN MQW as well as its bulk counterparts will be

D.9 6

evaluated. A full ab-initio treatment on the 3D irreducible Brillouin Zone wedge will be performed. This theoretical work could be directly confirmed by Raman experiments. We postulate that the decay rate is slower in the MQW than that in the bulk counterparts. This work would shed light on device designs in relevant fields and fill the knowledge gap for phonon decay in nano-crystals

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12:15 **Size effects in molecular dynamics simulations of thermal conductivity in isotope doped silicon** D.9 7

Authors : R. Frieling(1), M. Radek(1), H. Bracht(1), D. Wolf(2)
Affiliations : (1) University of Münster, Institute Of Materials Physics, D-48149 Münster, Germany; (2) University of Duisburg-Essen, Physics Department, D-47048 Duisburg, Germany

Resume : Due to its high thermal conductivity natural silicon is not suitable as a material for thermoelectric applications. Recent experimental studies demonstrate that the thermal conductivity of silicon is efficiently reduced by isotope doping without degrading the electronic properties. Non-equilibrium molecular dynamics simulations are performed to identify the isotope doping and/or isotope layer ordering with minimum thermal conductivity. A temperature gradient along the sample is established by adding an amount of heat to a group of atoms at the hot end of the sample, that represents the heat source, and subtracting the same amount of heat from another group of atoms at the cold end, that is the heat sink. The thermal conductivity is calculated from the added amount of heat per time step, the cross section area of the sample, and the steady state temperature gradient along the sample. In this kind of setup the predicted thermal conductivities depend on the size of the simulation cell due to phonon scattering at the interfaces between sample and heat source, respectively, heat sink. The effect of the simulation cell size on the thermal conductivity of isotopic alloys and superlattices is reported. Moreover, the impact of the superlattice periodicity and isotopic intermixing at the interfaces of the heterostructure on the thermal conductivity of silicon is discussed.

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12:30 Lunch break

Poster Session II : Jouni Ahopelto (VTT)

14:00 **Exciton-phonon coupling in monodisperse single crystalline anatase TiO2 nanotubes** D.P.2 1

Authors : Hyunjun Yoo, Myungjun Kim, Hyunchul Kim, Seonhee Lee, Changdeuck Bae, Hyunjung Shin
Affiliations : Dept. of Energy Science, Sungkyunkwan University, Suwon 440-746, Korea

Resume : Exciton–phonon coupling play a key role in carrier transport and charge recombination. Here we present that injected electrons are strongly coupled with phonons in tubular arrays of crystalline TiO2 in nanoscale. Photoluminiscence (PL) and Raman spectroscopy were performed for the understanding of their charge transport mechanism. The TiO2 anatase nanotubes' array is fabricated by template-directed atomic layer deposition (ALD) method. Dimensions of mono-dispersed TiO2 nanotube such as length, outer diameter, and wall thickness are precisely controllable and it is consisted of quasi-single crystalline elongated grains of anatase. Excitons are generated in TiO2 by external photons and they are immediately self-trapped in TiO6 octahedra with lattice distortion. Trapped excitons are transferred by hopping mechanism with self-trapping - detrapping processes with periodic energy losses. We observed periodic peaks in PL spectra with the energy difference of about 45 meV periodically. The periodic energy difference is closely matched to the optical phonons of anatase TiO2 represented with B1g(v4) in Raman spectra. As strong ionic bonded crystals with a soft phonon vibration (Eg), small polarons are expected in anatase crystals, unlike to Rutile. We observed fingerprints for the small polarons from our well organized, mono-dispersed and crystallized anatase nanotubes using low temperature - PL study. These observations strongly support small polaron hopping mechanism with longer life time in anatase crystals as photoanodes.

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14:00 **Thermal conductivity of suspended GeTe and Ge2Sb2Te5 nanowire measured by Raman spectroscopy with laser heating** D.P.2 2

Authors : Sungjin Park1, Dambi Park1, Kwangsik Jeong1, M. –H. Cho1*, Y Yi1, H. Kim2

and Bongyoung Yoo3
Affiliations : 1 Institute of Physics and Applied Physics, Yonsei University, Seoul, 120-749 Korea,2 School of Advanced Materials Science and Engineering, Sungkyunkwan University, Suwon 440-746, Korea, 3 Department of Materials Engineering Hanyang University, Ansan 426-791, Korea
Resume : GeTe and Ge2Sb2Te5(GST) nanowire were synthesized by using a vapor-liquid-solid method with GeTe and GST powder. The composition and crystalline structure of nanowires were confirmed by energy-dispersive spectroscopy (EDS) and high resolution transmission electron microscopy (HRTEM), respectively. The thermal properties of nanowires were confirmed by the optical method which uses laser heating and the determination of the local temperature by Raman spectroscopy. As temperature increased, the raman peaks are shifted to low frequency and broadened. To determine the value of thermal conductivity (κ), Finite-difference time-domain (FDTD) method for estimation of laser power absorbed in nanowire was carried out. The obtained thermal conductivity value of GeTe and GST nanowire is 3.88 Wm-1K-1 and 3.57 Wm-1K-1, respectively. Because these wires are nano-size and single crystal, the thermal conductivity values are higher than those of previous reports.

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14:00 **Engineering the Thermal Properties of CrAlSiN PVD Hard Coatings for Machine Tool Applications**

Authors : M. K. Samani 1,2,, L. Loisel 1,2,3, X. Z. Ding 4, N. Khosravian 1, G Chen 5, B. K. Tay 1,2,
Affiliations : 1 School of Electrical and Electronic Engineering, Nanyang Technological University, Nanyang Avenue, Singapore 639798 2 CINTRA CNRS/NTU/THALES, UMI 3288, Research Techno Plaza, 50 Nanyang Drive, Border X Block, Level 6, Singapore 637553 3LPICM (Laboratoire de Physique des Interfaces et des Couches Minces) UMR 7647, CNRS-Ecole Polytechnique, 91128 Palaiseau Cedex, France 4 Surface Technology Group, Singapore Institute of Manufacturing Technology, 71 Nanyang Drive, Singapore 638075 5 BC Photonics Technological Company 5255 Woodwards Rd., Richmond, BC V7E 1G9 Canada D.P.23

Resume : A series of about 3 µm-thick CrAlSiN coatings have been deposited using the lateral rotating arc technique. Their thermal properties have been measured using a pulsed photothermal reflectance setup. It is shown that the thermal conductivity decreases when the Al and Si content increases in the coating. Energy dispersive analysis of X-rays and X-ray diffraction were used to characterize the composition and the microstructure of the coatings, respectively. It was found that the size of the grains decreases as the (Al Si) content increases, hence leading to more phonon scattering. The conjugation of these results with those reported on mechanical properties would find potential application in the machine tool industry.

add to my program **(close full abstract)**

14:00 **A 1D PhoXonic Crystal**

Authors : J. Gomis-Bresco1, D. Navarro-Urrios1, M. Oudich2, S. El-Jallal2,3, A. Griol4, D. Puerto4, E. Chavez1,5, Y. Pennec2, B. Djafari-Rouhani2, F. Alzina1, A. Martinez4 and C. M. Sotomayor Torres1, 6.
Affiliations : 1 ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Campus UAB, 08193 Bellaterra (Barcelona), Spain 2IEMN, Universite de Lille 1, Villeneuve d'Ascq, France 3 PRILM, Universite Moulay Ismail, Faculte des sciences, Meknes, Maroc 3Nanophotonics Technology Center, Universitat Politecnica de Valencia, Valencia, Spain 5 Dept. of Physics, Universitat Autonoma de Barcelona, 08193 Bellaterra (Barcelona), Spain. 6 ICREA - Institucio Catalana de Recerca i Estudis Avancats, 08010 Barcelona, Spain D.P.24

Resume : Simultaneous confinement of light and sound in the same cavity generates a strong phonon-photon interaction, known as optomechanical (OM) coupling. Several optomechanical systems provided already proof of concept demonstrations for enhanced telecommunication devices and sensors. And using OM cavities, the basis for coherent phonon manipulation have already been set and/or propose. OM crystals (cavities built using the concepts of photonic and phononic crystals) target high frequency phonons. High frequency phonons have a competitive advantage as the thermal phonon population decreases with frequency. Using OM crystals, a recent work achieved a single confined phonon by OM cooling starting at moderate cryogenic temperatures. If the OM cavity is built using a complete phonon bandgap we calculated a better limitation of phonon losses, robust to fabrication imprefections. Cavities with simultaneous bandgap for light and sound are known as phoXonic crystals. We study the OM interaction in a 1D phoXonic crystal cavity. The cavity consists of a suspended

silicon nanobeam made with the repetition of a cell with a centered hole and a centered stub. A defect made by changing appropriately the cell dimensions towards the nanobeam center confines simultaneously light and sound. We present the experimental characterization of such structure, where we have detected by OM transduction modes inside the complete bandgap.

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14:00 **Microscopic description of coherent transport by thermal phonons** D.P.25

Authors : Benoit Latour, Sebastian Volz, Yann Chalopin

Affiliations : Laboratoire EM2C, Ecole Centrale Paris

Resume : By introducing a microscopic definition of the spatial phonon coherence length, we demonstrate using Molecular Dynamics simulations at equilibrium the existence of a coherent transport of thermal energy in superlattices. A criterion based on this coherence length is provided to distinguish this coherent transport regime from diffuse interface scattering. This approach gives a convenient framework for the interpretation of previous thermal conductivity measurements and calculations. It opens efficient strategies to design thermal properties of phonon systems at the nanoscale.

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14:00 **Steady State and Modulated Temperature Profiles in a Two-layer System Predicted by the Phonon Boltzmann Transport Equation** D.P.26

Authors : J. Ordonez-Miranda (1), Thomas Antoni (1,2), Yann Chalopin (1), and Sebastian Volz (1)

Affiliations : (1) Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion, UPR CNRS 288, Ecole Centrale Paris, Grande Voie des Vignes, 92295 Chatenay Malabry, France. (2) Ecole Centrale Paris, Laboratoire de Photonique Quantique et Moléculaire, CNRS (UMR 8537), Ecole Normale Supérieure de Cachan, Grande Voie des Vignes, F-92295 Chatenay-Malabry cedex, France.

Resume : The blossoming of nanotechnology involving the miniaturization of devices with enhanced rates of operation requires a profound understanding of their thermal performance. This is particularly critical in nanomaterials, in which the heat transport is not necessarily described by the Fourier?s law of heat conduction. In this work, based on the phonon Boltzmann transport equation under the relaxation time approximation, the steady-state and modulated temperature profiles inside a thin film in thermal contact with a semi-infinite layer are derived and analyzed, as a function of the film thickness and modulation frequency. By considering that the phonon mean free path and relaxation time are independent of temperature and phonon frequency, novel analytical solutions of the Boltzmann transport equation for the temperature and heat flux are obtained. It is shown that: 1) when the film thickness is much greater than the mean free path and for frequencies much smaller than the inverse of the relaxation time, the amplitude and phase of the temperature exhibit the diffusive behavior predicted by the Fourier?s law. By contrast, when this thickness is comparable to or smaller than the mean free path, these signals display attenuated oscillations, which become stronger as the film thickness decreases in nanoscales or the frequency increases in the range of THz. 2) The cross-plane thermal conductivity of a thin film increases with the ratio between the film thickness and the phonon mean free path, such that it reaches its bulk value when this ratio goes to infinity. This result is determined through an explicit expression for the thermal conductivity and it represents a more accurate extension of previous formulas reported in the literature [1,2]. This new approach allows us studying the heat conduction in the diffusive, diffusive-ballistic, and ballistic regimes, and it represents the theoretical framework to perform the microscopic characterization of nanofilms, through the determination of the mean free path and relaxation time of phonons. [1] A. Majumdar, ASME J. Heat Transfer 115, 7 (1993). [2] G. Chen, Phys. Rev. B 57, 14958 (1998).

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14:00 **Acousto-optic couplings in two-dimensional Lithium Niobate phoxonic crystal** D.P.27

Authors : Quentin ROLLAND. Samuel DUPONT. Joseph GAZALET. Jean-Claude KASTELIK

Affiliations : Institut d'Electronique, de Micro□electronique et de Nanotechnologie, UMR CNRS 8520, Universit□e de Valenciennes-Hainault-Cambresis, Valenciennes, France

Resume : We investigate the acousto-optic couplings in two-dimensional infinite piezoelectric phoXonic crystal cavities. The periodic structure considered consists in a square array of air inclusions drilled in Lithium Niobate matrix. This structure allows the simultaneous confinement of acoustic and optic waves in a point defect obtained by removing one hole from the structure. Our theoretical analysis takes into account three different coupling mechanisms. In addition to the traditional effects: photo-elastic effect and opto-mechanic effect existing in

non-piezoelectric materials, we consider the electro-optic effect introduced by the electric filed accompanying the phonon. Using the finite element method, we analyze the perturbation of the photonic cavity modes under the action of phononic cavity modes. We first discuss some aspects of the additional electro-optic effect. For illustration purposes, we compare the coupling strength of two analogous breathing modes, one as found in the LiNbO3 structure and another mode qualitatively comparable but evidenced in a similar silicon structure. Then, we end the discussion by an analysis of the coupling strength dependence on typical crystallographic cuts of Lithium Niobate.

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14:00 **Conversion of Laser Pulse Optical Energy to Photo-acoustic Wave in nm-Scale Layered TlGaSe2 Crystals**

Authors : K. Gulbinas (1), V. Grivickas(1), P. Grivickas (2), J. Linnros (3)
Affiliations : (1) Institute of Applied Research, Vilnius University, Vilnius, Lithuania; (2) Institute for Shock Physics, Department of Physics and Astronomy, Washington State University, Pullman, Washington, USA (3) School of ICT, Royal Institute of Technology, Kista-Stockholm, Sweden;

Resume : Experiments are presented that reveal an efficient optical energy conversion from the visible to the infrared wavelengths range as a result of photo-acoustic response (PAR) after light pulse incites onto the free surface of TlGaSe2 crystal. Excitation was carried out with a tunable wavelength of ns-pulse laser and the PAR was detected laterally with a focused cw-probe. When the excitation was directed perpendicularly to 2D crystal layers the acoustic wave traveled across the layers, a linear PAR increase over three orders of the excitation power was observed and reached up to 80 % of cw-amplitude. Within 1.5 - 2.5 eV excitation range the PAR maintained a constant signal shape and multiple acoustic echoes persisted on a millisecond time range which indicates good quality of 2D nm-scale layer stacking. The observed properties can be related to variety of successive factors: huge electron-hole-phonon deformation potential, the restricted carrier diffusivity across the layers (thus absence of surface recombination), a high factor of refraction coefficient dependency on acoustic pressure, the absence of the band filling effect, and the relatively low absorption coefficient due to close proximity of the forbidden direct-band and the allowed indirect-band optical transition. All these factors ensure that the acoustic energy remain well confined under a wide pulse power and wavelength range suggesting that TlGaSe2 is a promising material for dynamic optical energy conversion.

D.P.28

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14:00 **Modelling of the phonon attenuation in Si-based nanostructures**

Authors : E. Chavez-Angel, R.A. Zarate, F. Alzina, C. M. Sotomayor Torres
Affiliations : Institut Catala de Nanociencia i Nanotecnologia, ICN2, Campus UAB, 08193 Bellaterra (Barcelona), Spain. Dept. of Physics, Universitat Autonoma de Barcelona, 08193 Bellaterra (Barcelona), Spain; Departamento de Fisica, Universidad Catolica del Norte, Av. Angamos 0610, Antofagasta, Chile; Institut Catala de Nanociencia i Nanotecnologia, ICN2, Campus UAB, 08193 Bellaterra (Barcelona), Spain; Institut Catala de Nanociencia i Nanotecnologia, ICN2, Campus UAB, 08193 Bellaterra (Barcelona), Spain. Institucio Catalana de Recerca i Estudis Avancats, ICREA, 08010 Barcelona, Spain.

Resume : The phonon lifetime is an important parameter as it limits the performance of the quality factor, Q, of micro/nano-scaled resonators. Moreover, as has been above, they are a and is a necessary input parameter for accurate calculations of nanoscale thermal transport. The fundamental theory of the phonon lifetime is well established. However, the testing of these models with the experimental data has been challenging due to complexity of models themselves, the use of fitting parameters that still remains unknown, e.g. Gr? neisen parameter, and also due to the few experimental reports of phonon lifetime in the gigahertz and terahertz regime. In the present work, the intrinsic and extrinsic scattering mechanism in Si nanostructures is studied. The extrinsic mechanism is carried out considering surface roughness scattering. The effect of boundary scattering due to surface roughness may be introduced through a boundary condition on the steady-state Boltzmann transport equation[1]. The intrinsic sound absorption is calculated using two theoretical approaches: (i) Landau-Rumer or three-phonon scattering processes[2] and (ii) Akhieser mechanism or viscous damping mechanism[3]. References [1] J. M. Ziman, Electrons and Phonons: The Theory of Transport Phenomena in Solids. Oxford University Press, USA, 1960. [2] L. D. Landau and G. Rumer, Phys. Z. Sowjet., 11(1937), pp. 18. [3] A. Akhieser, J. Phys. USSR, 1(1939), pp 277

D.P.29

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14:00 **Simultaneously resonant optical and elastic waves for enhanced acousto-optic interaction**

Authors : N. Papanikolaou(1), E. Almpanis(1), N. Stefanou(2)
Affiliations : (1) Department of Microelectronics, IAMPPNM, NCSR "Demokritos", GR-15310 Athens, Greece. (2) University of Athens, Section of Solid State Physics, Panepistimioupolis, GR-15784, Athens, Greece.

Resume : Recently, there has been a growing interest in optically generated mechanical vibrations in optical cavities, which led to new perspectives in acousto-optic (AO) devices that create hypersound by light. This, so called, optomechanical coupling is due to the deformation induced by optical radiation pressure in a high-Q factor optical cavity that eventually generates elastic waves through a feedback mechanism. Moreover, recent reports on phonon driven optical processes like the stimulated Brillouin scattering in nanowires has renewed the interest on the AO interaction in the nanoscale. These advances, could open new perspectives towards light manipulation and information processing through phonons in optical circuits. High-frequency elastic vibrations, can be also used to manipulate light in structures that simultaneously sustain elastic and optical wave resonances in the same volume. We will address the problem of the AO interaction in structures that localize optical and elastic waves and discuss the consequences of the simultaneous confinement, as well as the limits of validity of the first order Born approximation usually used to describe the photon-phonon coupling in this case. Moreover we will consider the issue of losses and present few examples in simple one dimensional multilayer structures.

D.P.2 10

add to my program (close full abstract)

14:00 **Scanning Thermal Microscopy studies of 2D materials**

Authors : Benjamin J. Robinson, Peter D. Tovee, Oleg V. Kolosov
Affiliations : Physics Department, Lancaster University, Lancaster, LA1 4YB, UK

Resume : Measurement of thermal properties at the nanoscale presents a number if unique challenges. Here we report the exploration of the thermal properties of a range of 2D materials using scanning thermal microscopy (SThM) on the atomic thickness scale of ca. 0.3nm (monolayer) incrementally to bulk and the lateral resolution on the length scale of a few tens of nm. Materials include graphene, MoS2, Bi2Se3, GaTe, GaS and GaSe. SThM is a modification of the Atomic Force Microscope employing a self-heated probe which is bought into contact with the sample correspondingly causing a drop in the probe temperature which can be monitored and interpreted to estimate the sample's thermal properties. We have investigated how these properties change as a function of sample thickness for the range of 2D materials listed above on substrates of both high and low thermal conductivity. We observe well defined values of thermal conductance for monolayer and near monolayer thicknesses, however some materials show increased conductance at increasing multilayers whilst others show a decrease – in most cases the conductance does not scale simply with thickness. We will discuss experimental considerations and possible thermal conductance models to explain these interesting results and describe a new approach for thermal quantification – Force Spectroscopy SThM.

D.P.2 11

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14:00 **Spectral Detection of Surface Phonon-Polaritons propagating in Micro-sized Glass Tubes**

Authors : Laurent Tranchant1, J. Ordonez-Miranda1, Beomjoon Kim2, Thomas Antoni1,3, Yann Chalopin1 and Sebastian Volz1
Affiliations : 1 Laboratoire d'Energetique Moleculaire et Macroscopique, Combustion, UPR CNRS 288, Ecole Centrale Paris, Grande Voie des Vignes, 92295 Chatenay Malabry, France. 2 CIRMM, Institute of Industrial Science, the University of Tokyo, Japan. 3 Ecole Centrale Paris, Laboratoire de Photonique Quantique et Moleculaire, CNRS (UMR 8537), Ecole Normale Superieure de Cachan, Grande Voie des Vignes, F-92295 Chatenay-Malabry cedex, France.

Resume : Because of the disappearance of the convection at the nanoscale, nano-heat transfer can be supported only through conduction and radiation. The reduce system size yields a larger thermal resistance through conduction, but the larger surface to volume ratio leads to promising features for guided radiation. Indeed surface waves can be exalted thanks to the increase of their propagation lengths along the surface of nano-systems. Surface Phonon-Polaritons (SPPs) are one kind of these surface waves, which propagate in the ten microns range corresponding to the spectral range of blackbody radiation. Their energy density can be several orders of magnitude higher than the one of the propagating waves described by the Planck's law in the far field [1]. Besides, by augmenting the SPPs propagation length along the surface, we can raise the

D.P.2 12

effective thermal conductivity of polar dielectric nano-systems like glass nanotubes by a factor of two [2]. In order to support our calculations, we designed an experiment to measure the power and the spectral characteristics of thermally excited SPPs. However they are evanescent waves, which means that they cannot be simply detected in the far-field unless diffracted as in a SNOM set-up [3] or by a grating [4]. Here we use an original combination of both solutions by diffracting the SPPs by the tip of a glass tube, which has a diameter of the order of one micron. This tip effect allows us to measure the spectrum of SPPs propagating along the glass nanotube by using an IR microscope coupled with a FTIR spectrometer. The heating of the glass nanotube is carried out by focusing a 1 W green laser on a copper coating, which was deposited on the lower region of the glass tube. This setup enables us to get the spectrum and the power of the diffracted SPPs regarding to the temperature of the heated glass tip. [1] K Joulain, Microscale and Nanoscale Heat Transfer, Topics in Applied Physics (107), by S Volz (Ed.) 2007 [2] Ordonez -Miranda J. et al, Anomalous thermal conductivity by surface phonon-polaritons of polar nano thin films due to their asymmetric surrounding media, J. of App. Phys. 113, 084311 (2013). [3] Huber A., Ocelic N., Kazantsev D., and Hillenbrand R., Near-field Imaging of mid-infrared surface phonon polariton propagation, App Phys Lett 87, 081103, 2005. [4] Le Gall, J., Olivier, M., and Greffet, J.-J., Experimental and Theoretical Study of Reflection and Coherent Thermal Emission by a SiC Grating supporting a Surface Phonon Polariton, Phys Rev B 55, 10105, 1997.

14:00 **Study of thermoelectric effect in silicon nanowires within a full-band Monte Carlo approach**

Authors : Jérôme Larroque, Jérôme Saint-Martin
Affiliations : Institut d'Electronique Fondamentale, CNRS UMR 8622, Université Paris-Sud, Orsay, France

Resume : The quality of a thermoelectric material is quantified by its figure of merit ZT which is proportional to electrical conductance and inversely proportional to thermal conductance. As the mean free path of phonons is larger than the mean free path of electrons, the dimension of a device can be used to degrade the thermal transport while keeping good electrical performance. In this context, nanowires are promising thermoelectric architectures. In this work, phonon transport is studied in silicon and germanium nanowires within a Monte Carlo approach considering the full dispersion of phonons in the whole Brillouin zone. A semi-empirical method, the Adiabatic Bond Charge Model is used to estimate the dispersion of phonons in silicon. The anisotropy of phonon transport is preserved by this full-band approach. The main process of scattering phonons-phonons is the three phonons scattering which turns one optical phonon into two acoustic phonons and vice versa. But in the algorithm, a phonon which undergoes a piece of scattering is replaced with another phonon randomly selected [1] to respect the Kirchhoff law. The relaxation time approximation is used and the parameters are fixed according to the Holland's model. The devices studied by the algorithm are silicon nanowires with a width of some 100nm. The aim is to estimate the effect of lateral confinement and the effect of the roughness of surfaces on the thermal conductivity of the nanowires. [1] Phys. Rev. B 72, 064305 (2005)

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14:00 **Thermal properties of silver nanowire networks**

Authors : S. Sorel1, M. Lagrange2, D. P. Langley2,3, N. D. Nguyen3, Y. Bréchet4, D. Bellet2, J. N. Coleman1
Affiliations : 1 School of Physics, CRANN and AMBER, Trinity College Dublin, Dublin 2, Ireland. 2 Laboratoire des Matériaux et du Génie Physique CNRS - Grenoble INP, 3 parvis Louis Néel CS 50257, 38016 Grenoble, France. 3 Laboratoire de Physique des Solides, Interfaces et Nanostructures Département de Physique, Université de Liège Allée du 6 Août 17, B-4000 Liège, Belgique. 4 Laboratoire de Science et Ingénierie des Matériaux et des Procédés CNRS - Grenoble INP, 1130 rue de la piscine 38042 Saint-Martin d'Hères, France.

D.P.2 14

Resume : Silver nanowire (AgNW) networks have recently been the focus of intense research due to their potential use as transparent electrodes in solar cells, flat panel displays or transparent heaters. Metallic nanowire networks can be deposited using low-cost and scalable deposition techniques on flexible substrates. For improving the transport properties (thermal and electrical) and optical transmittance in the visible range, an optimum nanowire density should be considered. In the present contribution we investigate the thermal behaviour of AgNW networks based on two aspects. The first one shows that a thermal

annealing can drastically improve transport properties. The second approach investigates the physical properties of the network when used to generate heat. Experimental observation shows that AgNW networks exhibit the properties of a very efficient transparent heater, making them appropriate for future uses compatible with large area and flexible display technology. A comprehensive understanding of the thermal properties of this promising transparent nanostructured network will be presented. References: S. De, P.J. King, P. E. Lyons, U. Khan, J.N. Coleman. ACS Nano 4 (2010) 7064. D.P. Langley, G. Giusti, M. Lagrange, R. Collins, C. Jiménez, Y. Bréchet, D. Bellet, Solar Energy Materials and Solar Cells (2013) http://dx.doi.org/10.1016/j.solmat.2013.09.015 D.P. Langley, G. Giusti, C. Mayousse, C. Celle, D. Bellet, J.P. Simonato. Nanotechnology 24 (2013) 452001.

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14:00 **The Effect of Microstructure on the Thermal Conductivity of Nanoscale Polycrystalline AlN Thin-Films** D.P.215

Authors : Juliana Jaramillo; Wassim Kassem; Yann Chalopin; Emmanuel Ollier; Sebastian Volz

Affiliations : Laboratoire des Composants pour la Conversion de l'Energie, CEA; Laboratoire d'Energetique Moleculaire et Macroscopique, CNRS, Ecole Centrale Paris; Laboratoire d'Energetique Moleculaire et Macroscopique, CNRS, Ecole Centrale Paris; Laboratoire des Composants pour la Conversion de l'Energie, CEA; Laboratoire d'Energetique Moleculaire et Macroscopique, CNRS, Ecole Centrale Paris

Resume : In the process of understanding and developing a structured material permitting the modulation of phonon transport, we investigated how growth parameters influence microstructure and thermal conductivity of aluminum nitride (AlN) thin-films. Wurtzite AlN thin films were deposited by reactive RF and DC sputtering on Si(100) and Al2O3(0001) substrates. The influences of chamber pressure, N2 flow rate, applied power and substrate nature on deposition rate, crystalline structure and morphology of polycrystalline AlN thin-films were studied. The microstructure and texture of the films were characterized by X-ray diffraction and scanning electron microscopy. The experimental results showed that sputtering at a lower pressure leads to a higher deposition rate and a sufficiently high ion energy to form a textured AlN film with (002) preferred orientation. (002) crystallographic orientation is also enhanced with the increase in nitrogen (N2) concentration when maintaining a moderate applied power. Strong influence of the substrate on the growth mechanism of the AlN films was observed. The thermal conductivity was found to increase for strong fiber texture depending on the microstructure and growing conditions. Results regarding the influence of microstructure and preferred orientation on thermal conductivity of the material system are discussed.

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14:00 **Thermal corrections to the calculation of the thermal conductivity in suspended structures** D.P.216

Authors : P. Ferrando, A. F.Lopeandía, J. Rodríguez-Viejo

Affiliations : Nanomaterials and Microsystems Group. Physics dep. Universitat Autónoma de Barcelona. 08193 Bellaterra, Spain.

Resume : Suspended structures are widely used to measure thermal conductivity (k) on nanowires and thin films. Here we present a detailed analysis of the uncertainties in the measurement of thermal conductivity using suspended structures. These structures are often modeled using a 1D heat diffusion equation in order to extract the thermal conductivity of the sample under test. As we illustrate, the use of a 1D simplified model may give incorrect values of the thermal conductivity. To show this, we first calculate in a 1D approximation the uncertainty of the measured k value of the nanostructure for a wide range of thermal conductances. We prove the existence of a plateau with low uncertainties depending on the properties of the structure. Tuning these properties allows the fabrication of structures intended for the measurement of samples with specific thermal conductance. We have also carried out finite element modeling of the structure in 3D, to account for some inaccuracies that appear when k is calculated using the 1D equation for highly-conductive samples. In this framework, correct solutions of the thermal conductivity can be obtained for any geometry and/or thermal conductance.

add to my program (close full abstract)

14:00 **Monte Carlo simulation of micro-ribbon thermal conductivity at very low temperatures** D.P.217

Authors : Aymeric Ramiere (1), Jay Amrit (1), Sebastian Volz (2)

Affiliations : (1)Laboratoire d'Informatique pour la Mécanique et les Sciences de

l'Ingénieur UPR CNRS 3251,Université Paris-Sud, Rue John von Neumann,F-91403 Orsay, France; (2)Energétique Moléculaire et Macroscopique,Combustion, UPR CNRS 288, Ecole Centrale Paris, Grande Voie des Vignes F-92295 Chatenay-Malabry, France

Resume : We simulate a silicon micro-ribbon in contact with a large membrane at very low temperatures by using Monte Carlo technique [1]. Phonon-phonon interactions are neglected while a roughness of 4nm on the geometrical boundaries is considered. We show an increase of the ribbon effective thermal conductivity when the length decreases, which can be explained by the scattering specularity [2]. Influence of the membrane on the phonon energy spectrum and angle distribution at the end of the ribbon are also revealed. [1] R.B. Peterson, "Direct Simulation of Phonon-Mediated Heat Transfert in a Debye Crystal", Journal of Heat Transfert, vol 116, no.4, pp. 815-822, 1994. [2] A. Ramiere, J. Amrit and S. Volz, "Role of boundary roughness on heat transport in mesoscopic silicon ribbons at low temperatures", NanoEnergy Letters, no.6, pp. 13-14, 2013.

add to my program **(close full abstract)**

14:00 **Temperature dependence of Raman scattering in wurtzite GaAs nanowires: the functionalization effect with Au nanoparticles**

Authors : M. P. Leitão (2), M. R. Correia (1), B. P. Falcão (1), J. P. Leitão (1), Manuel Martins (2), Graça Pato, Sérgio Pereira (2), A. G. de Oliveira (3), F. M. Matinaga (3), J. C. González (3)
Affiliations : (1)Departamento de Física and I3N, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal; (2)CICECO and Departamento de Física, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal; (3) Departamento de Física, Universidade Federal de Minas Gerais, 30123-970 Belo Horizonte, Minas Gerais, Brazil

Resume : Semiconductor nanowires represent promising candidates for electronic, optoelectronic, sensor and thermoelectric applications. The knowledge of the vibrational properties of the GaAs nanowires is fundamental to understand the transport properties and the phenomena interaction with the free carriers, both of which have great impact on the device performance. Finite -size effects have in nanostructures are expected to modify the anharmonicity and the phonon decay times. This study involves samples of GaAs individual nanowires grown by molecular beam epitaxy (MBE) on GaAs (111)B substrates assisted by an Au catalyst, as well as GaAs nanowires whose surface was decorated with gold nanoparticles. Gold nanoparticles (diameter ~ 50nm) were synthesized in aqueous solution by a seeded growth strategy via the reduction of HAuCl4 with sodium citrate. Prior to nanoparticle deposition, the surfaces of GaAs nanowires were modified with a molecule, 1,3-propanedithiol, which acted as a linker allowing the assembly of gold nanoparticles to the GaAs nanowires surfaces. We report a systematical study of Stokes and anti-Stokes Raman scattering with the temperature (-196 ºC to 250 ºC).The temperature-induced changes of the vibrational properties of the nanostructures will be discussed before and after the functionalization with Au nanoparticles.

D.P.218

add to my program **(close full abstract)**

14:00 **Heat propagation and thermal phonon dynamics in group IV nanostructures**

Authors : M. R. Wagner, J. S. Reparaz, J. Gomis-Bresco, E. Chávez-Ángel, B. Graczykowski, F. Alzina, and C. M. Sotomayor Torres
Affiliations : ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Campus UAB, 08193 Bellaterra (Barcelona), Spain

Resume : The ability to control heat and phonon propagation at the nanoscale constitutes a key element for the realization of successful phonon engineering. The mean free path of thermal phonons Λ, which is the physical quantity determining the relaxation time τ of the thermal field, is still not accurately known for a wide range of technologically relevant materials such as e.g. silicon. Although some experimental and theoretical works suggest values for Λ in Si between 43 nm and 1 μm at 300 K, there is no conclusive evidence of its actual magnitude and temperature dependence. Furthermore, the lifetime of the thermal field τ has been only poorly determined. In this presentation, we address these issues by the investigation of the dynamics of low and high energy acoustic phonons using a two femtosecond laser pump and probe technique. The experiment is based on the asynchronous optical sampling method (ASOPS) which compared to standard pump and probe techniques provides a superior signal to noise ratio with a time resolution of about 50 fs. The pump beam locally creates a distribution of non-equilibrium phonons, whereas the probe beam is used to monitor the local temperature through the intensity of the transmitted light. This approach uses the large temperature dependence of the absorption coefficient exhibited by most semiconductors to

D.P.219

investigate the decay time of the thermal field. The presented results elucidate the frequency-resolved properties of the thermal field and thus contribute to paving the way towards smart heat management designs of nanostructures.

add to my program (close full abstract)

14:00 **Lifetime of high-order sub-THz thickness resonances in thin Si membranes**

Authors : A. A. Maznev, F. Hofmann, J. Cuffe, J. K. Eliason, K. A. Nelson
Affiliations : Dept. of Chemistry, MIT; Dept of Engineering Science, University of Oxford; Dept. of Mechanical Engineering, MIT; Dept. of Chemistry, MIT; Dept. of Chemistry, MIT

Resume : A suspended thin film that supports thickness resonances is the simplest kind of a high frequency solid state acoustic oscillator. Two most important characteristics of an oscillator are its frequency and damping time. While the frequency of thickness resonances can be easily obtained from the speed of sound and the plate thickness, the acoustic damping in thin membranes in the sub-THz range has not been explored until recent work [1], where lifetimes of fundamental thickness resonances of ultrathin Si membranes were reported. In this work, we focus our attention on high-order thickness resonances of Si membranes. Femtosecond laser pulses are used to excite and probe longitudinal acoustic wavepackets at a frequency of ~0.27 THz in suspended single crystal Si membranes with thickness ranging from 0.4 to 15 micrometers. The measured acoustic lifetime scales linearly with the membrane thickness and is shown to be controlled by the surface specularity which correlates with roughness characterized by AFM. Observed Q-factor values up to 2300 at room temperature result from a local maximum of the material Q in the sub-THz range. On the other hand, the measured specularity parameter of ~0.5 or less indicates that a negligible specularity would be expected at frequencies above ~1 THz. The results validate the use of the diffuse boundary scattering model in analyzing thermal transport in thin Si membranes. [1] J. Cuffe et al., Phys. Rev. Lett. 110, 095503 (2013).

D.P.220

add to my program (close full abstract)

14:00 **A NOVEL APPROACH TO NANOSTRUCTURING OF SnxSy THERMOELECTRIC THIN-FILMS USING LOW-COST SPRAY-DEPOSITION TECHNIQUE**

Authors : A. Ivaturi1, Firoz Alam2, Neetesh Kumar2, P. R. Bobbili1, N. Bennett1, J.-W. Bos3, V. Dutta2 and H. M. Upadhyaya1
Affiliations : 1Energy Conversion Laboratory, Institute of Mechanical Process and Energy Engineering, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom; 2Photovoltaic Laboratory, Centre for Energy Studies, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India; 3Institute of Chemical Sciences and Centre for Advanced Energy Storage and Recovery, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom.

Resume : Wide-scale waste-heat recovery via thermoelectrics (TEs) is most easily achievable for devices that combine low-cost raw materials with inexpensive fabrication processes. Tin sulphide has been identified theoretically as a very promising high-temperature TE material and crucially, is comparatively inexpensive compared to more traditional TE materials. In the present study, the TE properties of tin sulphide thin films and nanoparticle layers, deposited using indigenously designed large-area spray deposition system have been studied. Spray pyrolysis deposition is a relatively simple, industrially favoured and versatile method of making cost effective thin films on large areas. Here we present a systematic investigation of the doping properties of SnxSy thin films and nanoparticle layers subjected to novel nanostructuring route of post-deposition mechanical compression cycles as a function of the substrate temperature (250 – 450 ºC) and chemical composition of precursor solution. The samples have been characterised using TEM, XRD and SEM to study structure and morphology; Hall-effect measurements to study doping concentrations and hole mobilities. Seebeck coefficients, and electrical/thermal conductivities measurements are underway to demonstrate a novel and economical approach of nanostructuring by post-deposition mechanical compression as a promising route for enhancing the TE performance of SnxSy layers deposited by spray-pyrolysis.

D.P.221

add to my program (close full abstract)

14:00 **A Langevin approach to heat generated by Magnetic Nanoparticles**

Authors : Yann Chalopin, M. L. Beoutis, M. Devaud, S. Volz, F. Gazeau.
Affiliations : Laboratoire EM2C - Ecole Centrale Paris / CNRS. Laboratoire MSC - Univ. Paris Diderot / CNRS

Resume : This talk will present a microscopic study of the heating dynamics of magnetic nano-clusters in a biological environment. Our approach is based on

D.P.222

the solving of the Langevin equation adapted to a N-Body problem where the hamiltonian of the systems includes (local) magnetic dipole-dipole interactions in addition to an external magnetic field. By recovering the time fluctuations of each dipole at thermal equilibrium, we demonstrate how to predict the magnetic response of an aggregate. The corresponding heating efficiency is next studied through non-equilibrium simulations with an external magnetic field. The dynamics of the heat generated (dissipation) in the surrounding of the nanoparticle is computed from the work done by the dissipative forces acting on each magnetic particle. Our approach allows to correlate the size, shape, distribution and concentration of a magnetic aggregate to its heating capacity and provides a convenient tool to optimize hyperthermia for cancer treatments.

add to my program **(close full abstract)**

14:00 **POLYACETYLENE: RELATION OF THEORIES OF ELECTRICAL CONDUCTIVITY AND CHEMICAL REACTION IN THE SOLID**

Authors : K. BENOUMSAAD1; D. SAMSAR2; ILHEM. R. KRIBA2; A. DJEBAILI2
Affiliations : 1 Plasma Laboratory - Faculty of Sciences – Department of Physics- University of Batna- Algeria 2 Laboratory of chemistry and environmental chemistry L.C.C.E - University of Batna- Algeria,

Resume : The aim of this work was on the one hand the development of theoretical models (mathematical) to numerically simulate the experimental results of variations in the electrical conductivity as a function of various parameters, and on the other hand, the study of boundary conditions necessary for the numerical resolution of the heat propagation equation. Note that all obtained theoretical models are of the linear or sigmoidal form, Boltzmann type. Most obtained models allowed finding relationships more or less simple between the different parameters with an acceptable relative error of calculation, which allowed us to calculate theoretical values very close to the experimental values for the physical variables studied. Some of our models have given incorrect values , this can be explained by the fact that our calculation method is not reliable for this kind of data (values in small intervals). Note that this type of calculation can be improved by using other interpolation methods in particular the method of cubic splines. The model we have developed for solving the heat propagation equation, can serve in the research on the estimation of the isomerization temperature of PA by laser effect, which is widely used in current studies on the polyacetylene. Finally, it should be noted that our model for solving the heat propagation equation can be more efficient when the semi - empirical method is used to set the condition at the lower boundary of the domain.

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16:00 **PLENARY SESSION**

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Phonons and fluctuations in low dimensional structures

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start at	Subject	Num.
	Radiative Heat Transfer : Thomas Dehoux (U Bordeaux)	
09:00	**Manipulating the near field heat transfer between nanoscale objects by ultrathin layers** **Authors :** A. Kittel, D. Hellmann, K. Kloppstech, N. K?nne, and L. Worbes **Affiliations :** Physics Institute, University of Oldenburg, Germany **Resume :** Experimental investigations of the near field transfer down to sub-nanometer distances make an important contribution to the understanding of the involved mechanisms. A Near Field Scanning Thermal Microscope (NSThM) is able to image the heat transfer mediated by evanescent modes with a lateral resolution of a few nanometer. This instrument is the ideal instrument to investigate nanoscale objects in lateral extension and down to thicknesses of fractions of a nanometer. Evaporating ultrathin layers of different materials belonging to different material classes can influence the heat transfer even if the film is only a single atom layer. Clearly this has to be done under well-defined conditions to meet the needs usual in surface science which is the key for reliable and reproducible results. After sub-monolayers are deposited on the substrate their influence can by studied directly by imaging the heat transfer above little islands and their surroundings. Results from sub monolayer films of iron, iron oxide, water, organic die, and sodium chloride deposited on a substrate of Au(111) will be presented. By varying the film thickness ranging from a single layer to a few atomic layers the influence of film thickness can be studied. Already a single layer of the right material results in a pronounced increase of the heat transfer and, therefore, on the coupling of two nanoscale objects. add to my program (close full abstract)	D.101
09:30	**Application of the nonlocal macroscopic response theory of the dielectric function to the study of near field radiative heat transfer between two thermostatic dielectric materials** **Authors :** Farah SINGER, Younès EZZAHRI, Karl JOULAIN **Affiliations :** Institut Pprime, CNRS-Université de Poitiers-ENSMA, ENSIP, Département Fluides, Thermique, Combustion, Bâtiment de mécanique, 2 rue Pierre Brousse, F-86000 Poitiers. **Resume :** The application of the local model of the dielectric function to study the near field radiative heat transfer (NFRHT) between two semi-infinite parallel solid plane materials maintained at different temperatures and separated by a distance d, have shown that when d is of the order of or less than the shortest thermal wavelength, the heat flux diverges as 1/d^2 as d tends to zero. This increase is due to the tunneling contribution of the evanescent waves which adds to the contribution of the propagative waves of the far field at very small d. This divergence is a point of failure for the local theory. In our work, we use the nonlocal macroscopic response theory proposed by Halevi & Fuchs to study the NFRHT between two semi-infinite parallel planes of 6H- SiC. This theory takes into account the scattering of the electromagnetic excitation at the surface of dielectric materials, which leads to the need of additional boundary conditions to solve Maxwell's equations. These conditions appear as additional parameters in the expressions of the reflection coefficients. These parameters depend on the nature of the polarization of the electromagnetic field (Uy for S polarization, Uz and Ux for P polarization). The spatial dispersion effects are represented by an additional term depending on the square of the wave vector K in the expression	D.102

of the dielectric function. As different values are attributed to the parameters Ux, Uy and Uz, different expressions of the reflection coefficients in P and S polarization can be obtained. In all cases, we obtain saturation of the radiative heat flux when d tends to zero with the occurrence of very interesting features depending on the value of these parameters.

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09:45 **Heat Transfer between Polar Nanoparticles in the sub-10nm Gap Range**

Authors : Shiyun Xiong*, Kaike Yang**, Yuriy A. Kosevich*, Yann Chalopin*, Roberto D'Agosta**, Pietro Cortona***, Sebastian Volz*
Affiliations : *Laboratoire d'Energetique Moleculaire et Macroscopique, Combustion, UPR CNRS 288, Ecole Centrale Paris, 92295, Chatenay-Malabry, France **Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre Departamento Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain ***Laboratoire Structures, Proprietes et Modelisation des Solides, UMR CNRS 8580, Ecole Centrale Paris, 92295, Chatenay-Malabry, France

D.103

Resume : Heat transfer between two silica clusters is investigated by using the non-equilibrium Green's function method. In the gap range between 4 ? and three times the cluster size, the thermal conductance decreases as predicted by the surface charge-charge interaction. Above five times the cluster size, the volume dipole-dipole interaction predominates. Finally, when the distance becomes smaller than 4 ?, a quantum interaction where the electrons of both clusters are shared takes place. This quantum interaction leads to the dramatic increase of the thermal coupling between neighbor clusters due to strong interactions. This study finally provides a description of the transition between radiation and heat conduction in gaps smaller than a few nanometers.

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10:00 **Coffee break**

Nanoscale Thermal Transport II : Gyaneshwar Srivastava (U Exeter)

10:30 **Manipulation of heat transport in two-dimensional nanostructures**

Authors : Davide Donadio
Affiliations : MPI for Polymer Research Ackermannweg 10 55128 Mainz – Germany

D.111

Resume : properties of materials over a very wide range, and give access to physical phenomena that would not occur in three-dimensional systems. This is especially true for the vibrational porperties and the lattice thermal conductivity of materials. In this talk I will illustrate case studies of atomistic calculations of phonon transport in two-dimensional materials, namely graphene and ultrathin silicon membranes, in which the thermal conductivity can be modified over several orders of magnitude with respect to the respective bulk counterparts. In particular, non-Fourier thermal transport in graphene at non-equilibrium conditions, and how heat conduction may be affected by mechanical strain will be discussed. Whereas in the case of graphene dimensionality reduction leads to extremely high thermal conductivity, it will be also shown how modulating thickness and surface structure turn silicon nano-membranes into low-thermal conductivity systems, attractive for thermoelectric applications.

add to my program (close full abstract)

11:00 **Heat Transport along Nanofilms and Nanowires due to Surface Phonon-Polaritons**

Authors : Jose Ordonez-Miranda (1), Laurent Tranchant (1), Beomjoon Kim (1), Thomas Antoni (1,3), Yann Chalopin (1) and Sebastian Volz (1)
Affiliations : (1) Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion, UPR CNRS 288, Ecole Centrale Paris, Grande Voie des Vignes, 92295 Chatenay Malabry, France. (2) CIRMM, Institute of Industrial Science, the University of Tokyo, Japan. (3) Ecole Centrale Paris, Laboratoire de Photonique Quantique et Moléculaire, CNRS (UMR 8537), Ecole Normale Supérieure de Cachan, Grande Voie des Vignes, F-92295 Châtenay -Malabry cedex, France.

D.112

Resume : The blossoming of nanotechnology involving the miniaturization of devices with enhanced rates of operation requires a profound understanding and optimization of their thermal performance. This is particularly critical in nanomaterials, due to the significant reduction of their thermal conductance as their size is scaled down. The surface phonon-polaritons (SPPs) have shown wide potential to enhance the energy transport through these materials. The mean free path of these energy carriers can be much longer than that of phonons, however their contribution to the heat transport is not well understood

to date, especially in absorbing nanomaterials. In this work, the SPP contribution to the heat conduction along nanofilms and nanowires of different polar materials is investigated in detail. Based on the Maxwell equations, Boltzmann transport equation and Landauer formalism, it is shown that: (1) a small difference between the permittivities of the two media surrounding a nanofilm can generate large propagation lengths in the order of a few centimeters and therefore enhance remarkably the SPP thermal conductivity [1]. (2) The SPP energy transport in anisotropic nanofilms can be optimized by choosing the propagation direction along the direction of less energy absorption, decreasing the film thickness, increasing the film length and raising the temperature [2]. In these two cases, the SPP thermal conductivity can be higher than the one of phonons. (3) The SPP thermal conductance of polar nanowires is independent of the material characteristics and is given by pi^2kB^2T/3h, where kB and h are the Boltzmann's and Planck's constants, respectively and T is the temperature. This universal quantization holds not only for a temperature much smaller than 1 K, as is the case of electrons and phonons, but also for temperatures comparable to room temperature [3]. The experimental measurement of the SPP thermal conductivity and SPP thermal conductance is also explored by using infrared microscopy. The obtained results could have great applications in the thermal management of nanoscale electronics and photonics. [1] J. Ordonez-Miranda, L. Tranchant, T. Tokunaga, B. Kim, B. Palpant, Y. Chalopin, T. Antoni, and S. Volz, J. Appl. Phys. 113, 084311 (2013). [2] J. Ordonez-Miranda, L. Tranchant, B. Kim, Y. Chalopin, T. Antoni, and S. Volz, Appl. Phys. Express (In press). [3] J. Ordonez-Miranda, L. Tranchant, B. Kim, Y. Chalopin, T. Antoni, and S. Volz, Phys. Rev. Lett. (In press).

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11:15 **Thermal conductivity of encased graphene**

Authors : Jia Yang, Aaron J. Schmidt
Affiliations : Boston University

Resume : When graphene is supported by a substrate or encased between two materials, basal-plane heat transfer is suppressed by phonon interactions at the interfaces. We have used thermal waves to study encased graphene multilayers, obtaining simultaneous measurements of the basal-plane thermal conductivity and cross-plane thermal interface conductance for 1 -- 7 graphene layers encased between a metal and silicon dioxide. Comparison of multiple graphene samples indicates that phonon transmission into the substrate contributes to the reduction of basal-plane thermal conductivity. Our results have implications for heat transfer in two-dimensional material systems, and are relevant for applications such as graphene transistors and other nanoelectronic devices.

D.113

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11:30 **Thermal conductivity and thermal field distribution determination in free-standing Si and Ge membranes**

Authors : J. S. Reparaz, E. Chavez-Angel, M. R. Wagner, A. Shchepetov, M. Prunnila, J. Ahopelto, P. Vaccaro, I. Alonso, M. Garriga, A. R. Goñi, F. Alzina, and C. M. Sotomayor Torres
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Resume : We investigate the nature of the heat transport regime in a series of free-standing Si and Ge membranes using a two-laser Raman thermometry, a novel high resolution contactless technique for thermal conductivity determination and thermal field mapping. The experiments are based on creating a thermal distribution of phonons using a heating laser, while a second laser probes the local temperature through the spectral position of a Raman active mode of the membranes. We show that for 2-dimensional materials such as free-standing membranes or thin films, and for small temperature gradients, the thermal field decays as $T(r) \propto \ln(r)$ in the purely diffusive limit. The case of large temperature gradients within the membranes is also explored leading to an exponential decay of the thermal field, $T \propto \exp[-A \bullet \ln(r)]$. Furthermore, the influence of low dimensionality in the thermal transport regime is studied in a series of Si membranes down to 9 nm. We have observed a partial deviation from the diffusive thermal transport regime, which probably originates from phonon-phonon scattering suppression due to boundary scattering at the surface of the membranes. From these results we also give a rough estimation of the phonon mean free path at room temperature.

D.114

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11:45 **Measurement of phonon damping by nanostructures**

Authors : A. Al Mohtar, A. Bruyant, M. Kazan, J. Vaillant, A. Khoury.
Affiliations : University of Technology de Troyes, ICD-LNIO and STMR - UMR6279 CNRS, France; Applied Physic Laboratory (LPA), Faculty of Sciences II, EDST, Lebanese University, Lebanon; Department of Physics, American University of Beirut, Lebanon;

Resume : The understanding of phonon lifetime and scattering rates is attracting an increasing interest due to the major role of phonon in thermal and electrical conductivity that are key properties for technological applications. The infrared complex dielectric function of a crystal is determined by the harmonic characteristics of the phonon together with the intrinsic and extrinsic phonon scattering rates. In order to investigate the interplay between the phonon intrinsic scattering and the scattering of the phonon by a nanostructured surface, infrared reflectivity measurements from SiC nano-pyramids on SiC substrate has been analyzed using a Kramers-Kronig conversion technique to deduce the infrared complex dielectric function. Then, the real and imaginary parts of the dielectric function have been fitted simultaneously by using a theoretical model for the dielectric constant that considers frequency-dependent phonon damping at the center of the Brillouin zone. It has been found that surface nanostructuring strongly enhances the overall scattering rate of the phonon at the Brillouin zone center.

D.11 5

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12:00 **The thermal conductivity of modulated nanowires by Monte Carlo estimation of the phonon free paths**

Authors : Nikolaos Cheimarios 1,2 ; Xanthippi Zianni 1,3,4; Patrice Chantrenne 4
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Resume : Good thermoelectric materials require high electron power factor and low thermal conductivity. Recent theoretical predictions and observations have provided evidence that inhomogeneities can favor the thermoelectric properties of nanowires. Enhanced thermoelectric power factor has been observed in InAs nanowires at low temperatures and has been attributed to quantum effects in the presence of inhomogeneities. The thermal conductivity of nanowires is reduced by inhomogeneities. In an earlier work, we showed theoretically that the thermal conductivity of a nanowire can be more significantly reduced by diameter modulation than by diameter decrease. The calculations were done using a kinetic theory model based on the Boltzmann transport equation and the relaxation time approximation. The mean free path was estimated using the Matthiessen rule with the bulk mean free path and an average phonon-boundary scattering length. Here, we use a method earlier proposed to study the thermal conductivity of a nanostructure with arbitrary geometry through Monte Carlo sampling of the free paths associated with phonon-phonon and phonon-boundary scattering. The two methods are compared for various nanowire dimensions and geometry modulations.

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12:15 **Tailoring thermal conductivity of graphene via defect-and-molecular engineering**

Authors : Stefan Bringuier, Jean-François Robillard, Pierre Deymier, Krishna Muralidharan
Affiliations : Department of Materials Science and Engineering, University of Arizona, Tucson, AZ 85721; Institut d'Electronique, de Microélectronique et de Nanotechnologie, UMR CNRS 8520, Cité Scientifique, 59652 Villeneuve d'Ascq Cedex, France; Department of Materials Science and Engineering, University of Arizona, Tucson, AZ 85721; Department of Materials Science and Engineering, University of Arizona, Tucson, AZ 85721

Resume : The exceptional thermal properties of graphene have attracted enormous interest over the past decade. Consequently, there is an increased push towards utilizing graphene in thermal-management systems such as thermal interface materials and thermoelectrics. While, many recent investigations have demonstrated the ability to dramatically reduce thermal conductivity by molecular functionalization or by the introduction of structural defects, so far, the ability to enhance thermal conductivity of graphene has not been successfully demonstrated in a controllable fashion. For the first time, using robust atomistic simulation techniques such as molecular dynamics (MD) that use spatially resolved heat-current auto-correlation functions and spectral energy density analysis, we show that graphene's thermal conductivity can be

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suitably tuned to be either higher or lower, by the introduction of structural defects such as vacancies and by proper functionalization of the graphene sheet. Specifically, by varying the periodicity and density of structural defects as well as adsorbed molecules such as C60, we show that the thermal conductivity can be enhanced by up to 10 % and reduced by much larger percentages. In particular, the ability to enhance thermal conductivity is attributed to an increase in optical phonon lifetime, as a result of suppression of out-of-plane phonon-modes and coherent scattering effects, while the reduction in thermal conductivity is primarily attributed to boundary-scattering.

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12:30 **End of Symposium D**

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