MRS - F13 Symposium UU

Phonon Interaction Based

Materials Design -
Theory, Experiments, and

Applications

First talk today at 9 am

Boston, December 2-5, 2013

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Phonon Interaction Based Materials Design --Theory, Experiments, and Applications

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CONCLUDING REMARKS

Subhash Shinde, Sandia Labs

<u>Gyaneshwar P Srivastava</u> University of Exeter, UK

David Hurley, Idaho National Lab

Masashi Yamaguchi, Rensselaer Poly Inst, NY

5 Dec 2013

Our effort on phonon symposia

MRS Fall 2007 Symposium EE: Phonon Engineering – Theory and Applications (1.5 days + poster)

MRS Fall 2009 Symposium CC: Phonon Engineering for Advanced Materials Solutions – Theory and Applications (4 days + poster)

MRS Fall 2011 Symposium W: Phonons in Nanomaterials – Theory, Experiments, and Applications (4.5 days + poster)

MRS Fall 2013 Symposium UU: Phonon Interaction
Based Materials Design -Theory, Experiments, and Applications

(3.5 days + poster)

Theme set out for this symposium

To address fundamental and experimental issues related to phonon interactions and transport in structures representing <u>multiple</u> <u>length scales</u> (i.e. nano-materials, mesoscopic systems, bulk materials)

To address current concepts in phonon engineering to enable novel design and materials based solutions in technologically important areas

Phonon modes and dispersion relations

Experimental and theoretical studies of phonon dispersion relations for bulk, thin films and nanostructures using a variety of techniques.

Noted that current state-of-art DFT calculations do not reproduce neutron scattering data for phonon dispersion relations in UO2

Phonon thermal transport -- bulk materials

Lattice thermal conductivity calculations using both phenomenological theories (Boltzmann transport equation based and MD simulations) and ab-intio (DFT-based) methods.

Ballistic and coherent heat conduction.

Non-Fourier thermal transport.

Extremes of heat conduction in molecular materials.

Phonon thermal transport -- nano materials

Methods developed for bulk materials extended for nano materials.

Experimental results presented employing different techniques, e.g. 3ω method, thermoreflectance (TDTR, FDTR) and coherent phonon spectroscopies.

Results for thin films, self-assembled monolayers.

Effect of interfacial adhesive layers on thermal conductivity. Ballistic and coherent heat conduction.

Phonon related device applications

GaN electronics; Sasers; Excitonic devices; Quantum cascade lasers; Integrated photonic devices

Challenges to be met

Accurate, reproducible measurements of interface (Kapitza) thermal resistance

Theoretical treatments of: phonon boundary scattering; interface scattering; interface resistance; anomalous anharmonic scattering (such as in PbTe); anharmonic scattering in nanocomposites

Many others ...

Thank you

Huge thank you to all participants for their valuable contributions, making this series of symposium such a success and helpful to young researchers.

Best wishes for further successful symposia involving the role of phonons ...

QuickTime™ and a TIFF (LZW) decompressor are needed to see this picture.