## 21COE Programme: Mechanical Systems Innovation Open Seminar

21COE Programme: The Mechanical System Innovation Open Seminar 2007 will be held as follows. Professor Pawel Keblinski is a world leader of nano-scale thermal engineering through his atomic-level computational methods and theoretical analysis to study structure-property relationships. He is well-known for excellent studies on modeling of mechanical response and thermal transport in nano-structured materials, nanocomposites and nanofluids and other interfacial materials. Do not miss this chance to hear his talk in Tokyo. Participants from any departments or outside of The University of Tokyo are welcome.

## Invited Speaker: Professor Pawel Keblinski

(Materials Science and Engineering Department, Rensselaer Polytechnic Institute) (Currently Sabbatical Leave to Department of Physics, National University of Singapore)

## Title: Are interfaces good or bad for thermal management?

-- Mediocre carbon nanotube composites and ultra-low thermal conductivity solids --

Date & Time: December 11 (Tue) 13:30-15:00

Place: The University of Tokyo, Engineering Building II, 3rd Floor, Room 2-31A Map: http://www.u-tokyo.ac.jp/campusmap/cam01\_04\_03\_e.html

## Abstract:

When the microstructural feature, such as grain size in nanocrystalline materials or fiber diameter in nanocomposites, becomes comparable with the mean free path of the phonon (heat carrying thermal wave) the thermal transport is determined by thermal properties of interfaces rather than by bulk thermal conductivities.

In the case of carbon nanotube (CNT) polymer composites and suspensions interfaces play a detrimental role and severely limit the effective conductivity of the material due to large interfacial thermal resistance. Using a combination of modeling techniques including atomistic simulations, finite element analysis and homogenization theories, we will (i) demonstrate the physical origin a large interfacial thermal resistance between CNTs and soft media, (ii) explain why the thermal transport in CNT composites does not shows a signature of percolation and (iii) suggest possible solutions that maximize thermal conductivity of CNT composites.

In the quest for better thermally insulating materials interfaces can greatly help and allow to beat low thermal conductivity limits of amorphous or alloy materials. Using molecular dynamics simulations and phonon analysis we will show that the introduction of grain boundaries into layered crystals can explain recent experimental results on ultra low thermal conductivity (0.05 W/m-K) of WSe<sub>2</sub> crystals. Furthermore, we predict that introduction of mass disorder lead to a complete localization of phonons and further lowers thermal conductivity to about 0.01 W/m-K at room temperature, which is well below values characterizing still air.

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