# AEROSPACE & MECHANICAL ENGINEERING

## 2009 COLLOQUIUM 2010

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**INFORMAL COFFEE PERIOD BEFORE THE SEMINAR IN ROOM 365, ENGR. BLDG.**

**UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA 46556**


**SPEAKER:** **Jose A. Pascual-Gutierrez**
Purdue University
West Lafayette, Indiana


**TOPIC:** **ON THE THEORY OF PHONONS: A FUNDAMENTAL JOURNEY FROM THEIR ORIGINS TO THE INTRICATE MECHANISMS OF THEIR TRANSPORT**

**DATE:** Thursday, April 1, 2010

**TIME:** 3:30 p.m.

**PLACE:** 126 DeBartolo Hall


**ABSTRACT**

Phonon theory,originally given an identity following in the footsteps of electromagnetic theory, emerged as a necessity to explain the high thermal conductivity of crystallographic materials, yet remained overshadowed by electrons and photons and did not receive much attention by the electronic industry. In the last decade, however, the chip-based electronic industry, determined to deliver on its promise to increase transistors' integration density, has seen thermal-management issues escalate to become the industry's biggest challenge. CMOS are already in the sub-50 nm silicon technology and significant thermal transport reduction is experienced due to phonon confinement, which translates into a reduction of phonon group velocities. Moreover, proposed novel transistor designs in SOI-type structures such as FinFETs, while showing improvements in electrical performance, create additional thermal dissipation due to a significant increase of phonon correlated scattering in the channel region. The lack of phonon transport simulation tools by the industry faced with these thermal challenges has brought phonon theory into the spotlight.

This presentation will provide an overview of phonons in non-metallic materials and of the intricate mechanisms involved in their transport. Three main topics will be discussed:

1. Based on the results yielded by lattice dynamics in the harmonic approximation, it will be shown how size reduction affects the phonon spectrum of silicon. Additionally, the differentiation between quantum-confinement and size-confinement effects will be clarified.
2. Quantifying scattering rates has always been a daunting task for phonon theorists in their attempt to use Fermi's Golden Rule of perturbation theory of quantum mechanics. Although the equations of perturbation theory are very well outlined, their use to evaluate phonon scattering rates has been frustrated by the computation of the anharmonic interatomic force constants (IFCs) to the extent that attempts to quantify these anharmonic IFCs have resorted to approximations that far exceed the inherent approximations of perturbation theory. Equally important as this oversight has been the approximations employed to find the phase space of phonons participating in scattering events. Here, a methodology will be presented to accurately find the phase space of interacting phonons. In addition, Fermi's Golden Rule is successfully implemented without the need of approximations to compute the scattering rates of three-phonon processes.
3. The Boltzmann Transport Equation (BTE) is best suited to describe phonon propagation in non-metallic materials when the transport can be construed in terms of wave packets. However, due to the inherent complexity of expressing the inter-phonon collision term, phonon BTE solutions depend on relaxation time-like approximations. Under such approximations, quasi-equilibrium conditions are a must and inter-phonon collisions are expressed via heuristic arguments. In this talk a full-band Monte Carlo approach is introduced as an alternative path-to-solution to the BTE, offering an ideal framework for incorporating all inter-phonon collisions. This Monte Carlo approach offers a degree of insight and granularity into phonon transport not achievable under relaxation time approximations, even in highly non-equilibrium conditions. Further applications and extensions of this work will also be discussed.


**NOTE:** ***If you are interested in meeting individually with Jose Pascual-Gutierrez, please contact Evelyn at 631-5431***