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

UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA 46556

SPEAKER: **Mr. Vikas Tomar**
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TOPIC: **MULTI-SCALE MECHANICS OF MICROSCOPIC AND NANOSCOPIC CERAMIC COMPOSITES: A MATERIAL DESIGN PERSPECTIVE**

DATE: Thursday, April 14, 2005

TIME: 3:30 p.m.

PLACE: 317 DeBartolo Hall

Abstract

Nature has imposed severe restrictions on humans in terms of discovery of new elements to be added to the periodic table of elements. The best choice in terms of advancement of materials science therefore is to combine the properties of available elements using the most appropriate chemistry to obtain the most suitable physics and use sophisticated mathematics to add predictability. A branch of this schema adheres to the philosophy of closest possible control by going smaller and smaller in length as well as time scale. The computational mechanical implication of this branch manifests itself in form of the areas of *nanomechanics* and *micromechanics* focusing primarily on predictability and engineering performance issues of nanoscopic and microscopic material morphology, respectively. Within this scope I will primarily talk about my work on *nanomechanics* of α-Fe_2O_3+fcc-Al structural energetic nano-composites and nanointerfaces and *micromechanics* of TiB_2+Al_2O_3 ceramic composites. Primary tools used include, solid state physics and chemistry, classical molecular dynamics (MD), statistical mechanics, continuum mechanics, cohesive finite element method (CFEM), high performance computing, and scientific visualization. The research question answered is: what is the effect of morphological manipulations on the desired mechanical/multi-functional performance at the required range of loading? The issues analyzed include effect of phase morphology, phase distribution, and phase sizes on mechanical properties such as elastic constants, flow stress, and fracture strength and the effect of correlation between a material's morphology and the type of loading on the failure of a material. Both actual as well as idealized phase morphologies are used during the analyses. Two independent frameworks based on classical MD and second order perturbation CFEM, respectively, are developed and used. Ongoing efforts to integrate these analyses in form of a material design activity are elucidated. Future research directions in the multi-scale mechanics of nanomaterials and the design of nanomaterials are also discussed.