IUPUI DEPARTMENT OF MECHANICAL ENGINEERING
SCHOOL OF ENGINEERING AND TECHNOLOGY
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DEPARTMENT OF MECHANICAL ENGINEERING
Purdue School of Engineering and Technology

FALL 2008 SEMINAR SERIES

Date: Thursday, November 13, 2008
Time: 11:00 am – 12:00 pm
Room: SL 165

Everyone is invited

Computational Materials Design for Aluminum Dry Machining and Quick Plastic Forming

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Abstract.
Demands for light weight and fuel efficient automobiles have led to a steady increase in the use of aluminum alloys for structural components, however the low formability and active surface adhesion of aluminum still raise many challenges in forming and machining of aluminum alloys. In this talk, I will give examples on how atomic modeling combined with microstructure modeling and experiments to solve engineering problems and guide material design. First, I'll show a multiscale modeling approach for Quick Plastic Forming of Aluminum. Molecular Dynamics (MD) simulations of grain-boundary sliding (GBS) in aluminum suggested the existence of a threshold stress for GBS. The threshold stress was then included to improve the microstructure plasticity modeling. Finally the simulated stress-strain curves were used to simulate forming of aluminum parts. Consequently, material design can be done at both microstructure and grain boundary level. In solving the aluminum adhesion problem, Density Functional Theory (DFT) was used to directly provide insights and guidance for the coating design on the machining tools. To enable the nano-crystalline diamond coating for aluminum dry machining all three interfaces need to studied: adhesion transfer of Al to the coating surface is minimized; grain boundaries inside the coating is modified to reduce residual stress; and the coating/substrate interface is optimized to enhance the adhesion of the coating. These calculations served as initial steps towards designing new materials and solving engineering problems through multi-scale physics based modeling approach.

About the Speaker.
Dr. Yue Qi is a Staff Research Scientist working on computational materials sciences at Materials and Processes Lab, General Motors R&D Center. Her research spans hard coatings, light weight alloys, proton exchange membranes, and various nano-structured materials for energy storage. She completed her B.S. degree (Materials Science and Computer Science) at Tsinghua University, China in 1996. She received her PhD in Materials Science (minor in computer science) from California Institute of Technology in 2001. She then joined GM as a Sr. Research Scientist. She received 2006 GM Campbell Award for "Advances in Nano-scale Plasticity". She was the corecipient of 1999 Feynman Prize in Nanotechnology for Theoretical Work with Dr. T. Cagin and Prof. W. A. Goddard III (PhD advisor).