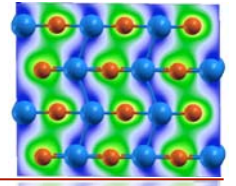


# Computational Materials Science Seminar



## Rate dependence of dislocation nucleation processes predicts twinning trends in f.c.c. metals

**Speaker: Professor Derek Warner**

**School of Civil and Environmental Engineering, Cornell University**

**Duffield 254, 2:00-3:00pm, Thursday, April 24**

### **Abstract:**

Increasing evidence indicates that dislocation nucleation plays a key role in the deformation of nano-structured and nano-dimensioned metals. Yet, our understanding of the nucleation process, whether it is from a free surface, grain boundary, or stress concentration, has remained clouded. Atomic simulations of these materials often show an excessive amount of twin emission and/or non-successive partial dislocation emission compared to experiment. We resolve this discrepancy by considering the thermally-activated nature of dislocation nucleation.

Our multiscale technique for long-time atomic simulations of crack tip behavior shows that in Al a transition from twinning at very short times and high applied loads to dislocation slip at longer times and lower applied loads. Twinning in Al is thus very rare, in agreement with experiments. We then develop an analytic model for the twinning/dislocation-slip competition that predicts dislocation slip to become the preferred mode of deformation with a lower activation energy at lower load levels, corresponding to longer times or slower loading rates, and/or higher temperatures, in agreement with our simulations. Moreover, this transition in mechanism is predicted to occur in all FCC metals, and the difference between materials then lies in the activation energy at which the transition occurs. Our ranking of FCC materials with respect to twinnability matches experimental trends, and captures both the temperature and loading-rate dependence.

To study twinning versus dislocation slip via simulation, a multiscale method is essential in overcoming severe computational hurdles. The finite-temperature concurrent multiscale Coupled Atomistic Discrete Dislocation (CADD) method minimizes the number of explicit atoms in the computational cell without affecting physical results while reducing the total CPU time to ~11 CPU years. Combining this technique with the parallel replica method enables MD simulations approaching one microsecond.

**Host:** Richard G. Hennig **Organizers:** T. Arias, G. Chan, R. Hennig, C. Umrigar

The Computational Materials seminars are held on the 1<sup>st</sup> and 3<sup>rd</sup> Thursdays of each month and provide an informal setting for internal and external speakers to present works on materials simulation and other theoretical aspects of materials.

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