

# Mechanical and Aerospace Engineering

## MAE Seminar Series

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### **High Temperature Wetting in Metal Systems: Insights from Atomic Simulations**

#### **ABSTRACT**

Molten metals are atomic liquids with relatively simple structure. Despite this, capillary phenomena for these systems typically involve reactions between the liquid and the solid on which the liquid wets. Such reactions are often exploited to develop strong mechanical bonds between two metals or a metal and a ceramic during technological processes including soldering and brazing. These joining processes have been employed for hundreds of years yet fundamental mechanisms dictating reactive spreading kinetics remain unclear. This talk will present results from molecular dynamics simulations of liquid Cu infiltrating a pore in solid Ni. The binary phase diagram for this system exhibits solid solution character and, accordingly, Ni dissolves into Cu(l) as the liquid moves down the pore. For relatively lower temperature, substrate dissolution is not aggressive and infiltration kinetics are well described by a Lucas-Washburn expression for capillary driven pore imbibition. However, for higher T, dissolution is significant such that infiltration kinetics cannot be described via standard capillary imbibition theory. To reconcile these results, a term was added to the Lucas-Washburn expression, representing the energy due to the dissolution reaction. Thermodynamic calculations demonstrate an Arrhenius dependence of the magnitude of this term, explaining the significant temperature dependence observed. The physical significance of the modified kinetic expression will be discussed along with a proposed alternative view on the role that dissolution has in determining capillary infiltration kinetics.

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Friday, October 16, 2009  
206 Furnas Hall  
11:00 am – 12:00 pm

