Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Kinetics and equilibrium properties of supercooled salt solutions in contact with ice and water vapor MARCELO CARIGNANO, PAUL SHEPSON, IGAL SZLEIFER, Purdue University — The kinetics of ice growth from salt solutions and the final equilibium systems are studied by Molecular Dynamics simulations. Two systems are investigated. In one a liquid layer of supercooled salt solution is sourronded by ice walls. In the other, the liquid layer is in contact with an ice block on one side and water vapor on the other side. We found that the kinetics of ice growth in both cases is slower than the corresponding system with no ions. A faster ice growth is obserbed on the prismatic plane than on the basal plane of the ice. In the cases where complete freezing is achieved, the final systems have all the ions participating in cluster formations. In the system with water/vapor interface, complete freezing is not reached, leaving the ions solvated in a quasi liquid layer. The density profiles of the ions show their preference to be closer to the water/ice interface than to the water/vapor interface. The simulations enable the understanding of the mechanisms for ice formation under different solution conditions, and the final equilibrium properties of the studied systems.

Marcelo Carignano
Purdue University

Date submitted: 11 Jan 2006 Electronic form version 1.4