Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Multiscale modeling of nanofoams under irradiation[1] E.M. BRINGA, CONICET & Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Argentina, J. RODRIGUEZ-NIEVA, Instituto Balseiro, Universidad Nacional de Cuyo, Argentina, J.D. MONK, Cain Department of Chemical Engineering, Louisiana State University, J.A. CARO, Los Alamos National Laboratory, M.J. LOEFFLER, NASA Goddard Space Flight Center, Astrochemistry Branch, Code 691, T.A. CASSIDY, CalTech/JPL, R.E. JOHNSON, R.A. BARAGIOLA, Laboratory for Atomic and Surface Physics, University of Virginia, D. FARKAS, Department of Materials Sciences, Virginia Tech — Nanoscale porosity appears in solids under a number of conditions: radiation damage in nuclear reactors, initial stages of ductile failure, in astro-materials, etc. Using molecular dynamics (MD) simulations, we analyze the radiation damage and surface modification of materials with various nanoscale porosities, where experimental techniques can be difficult to use and interpret. We consider (a) irradiation with ions with energies in the range 1-25 keV, of interest for fusion and fission energy applications; (b) swift heavy ion irradiation, with energies up to few GeV, relevant for track formation and interstellar grain evolution. We find that irradiation effects have larger spatial extent than for full-density solids and include the production of point-defects and twins which change the mechanical properties of the samples. We use our MD results as input for a Monte Carlo (MC) code to calculate sputtering yields from nanofoams of different geometries under different irradiation conditions. We also use our MD results to build models which predict possible radiation endurance under intense irradiation.

[1]E.M. Bringa thanks support from PICT2009-0092

Eduardo Bringa
CONICET & Instituto de Ciencias Basicas,
Universidad Nacional de Cuyo, 5500 Mendoza, Argentina

Date submitted: 29 Nov 2011 Electronic form version 1.4