Exascale Molecular Dynamics for Nuclear Materials

11/05/16

The goal of this project (led by Los Alamos National Laboratory, in collaboration with Sandia National Laboratories and University of Tennessee) is to stand up an exascale-ready molecular dynamics simulation code. This "EXAALT" code (Exascale Atomistics for Accuracy, Length, and Time) will allow users to reach currently inaccessible regions in the space of accuracy, length, and time, necessary for solving critical problems in materials science. A capability appropriate for two key problems in nuclear energy will be targeted: Understanding and controlling fission gas bubbles in fission nuclear fuels (FIG. 1), and understanding the formation of "fuzz" on the surface of tungsten under fusion plasma conditions (FIG. 2).

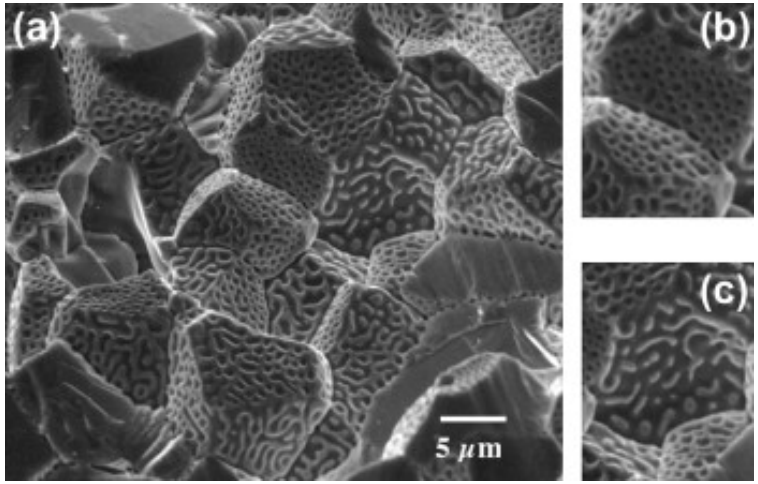

FIG 1: Scanning electron microscope images of fracture surfaces of UO_2 illustrating coalescence of fission gas bubbles on grain boundaries. Valin et al., *Proceedings of the Seminar on Fission Gas Behavior in Water Reactor Fuels*, NEA (2000).

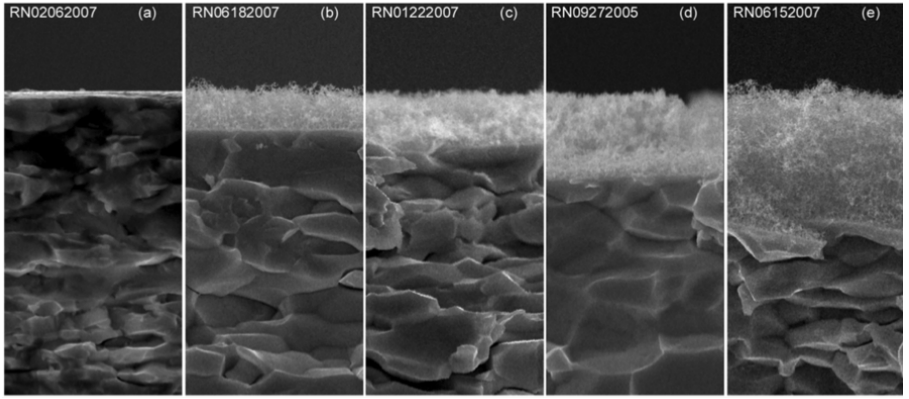

FIG 2: Nanoscale fuzz evolution on tungsten surface exposed to He plasma at T=1120 K, similar to fusion conditions. Tungsten is slated to be the first-wall material in planned fusion reactors. Figure from Baldwin and Doerner, Nucl. Fusion **48**, 035001(2008).