Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

The hydriding resistance of plutonium oxides and mononitride: A view from *ab initio* molecular dynamics[1] BO SUN, HAIFENG LIU, HAIFENG SONG, Institute of Applied Physics and Computational Mathematics, CAEP — Based on the non-local van der Waals density functional (vdW-DF)+U scheme, we carry out the *ab initio* molecular dynamics study of the interaction dynamics for H2 molecules impingement against Pu-oxides and mononitride surfaces. We show that except for the weak physisorption, both PuO2 and PuN surfaces are so difficult of access that almost all of H2 molecules will bounce back to the vacuum when their initial kinetic energies are not sufficient. Although the dissociative adsorption of H2 on PuO2 surfaces is found to be exothermic, the collision-induced dissociation barriers of H2 are very high (up to 2.2 eV). However, PuO2 overlayer on Pu-metal can be reduced to α-Pu2O3 drived by oxygen-lean conditions, and H2 can penetrate and diffuse in α-Pu2O3 easily. As a result, α-Pu2O3 can promote the hydriding process of Pu. Unlike PuO2, PuN is found to be one kind of stable and uniform passivation layer against Pu-hydriding. Specifically, the incorporation of PuN and H-atom is proven to be thermodynamically unstable. Overall, our current study reveals the mechanical and chemical resistances of Pu-oxide and Pu-nitride to hydrogen corrosion, which have strong implications to the understanding of the surface corrosion and passivation of Pu metal.

[1] This work was supported by the FDST of CAEP under Grant No. 9090707.

Bo Sun
Institute of Applied Physics and Computational Mathematics, CAEP

Date submitted: 22 Jan 2015 Electronic form version 1.4