Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Nucleation of aluminum nanoclusters on graphene: an ab-initio molecular dynamics study SUFIAN ALNEMRAT, Naval Postgraduate School, DENNIS MAYO, SAMANTHA DE CARLO, BRYAN EICHHORN, University of Maryland, JOSEPH HOOPER, Naval Postgraduate School — Recent experimental results have shown that liquid AlCl and AlBr can, in the presence of a reducing agent, nucleate and grow 10-20 nm aluminum nanoparticles on functionalized graphene sheets. This may offer a route to patterned 2D structures of Al nanoparticles and clusters. Here we present DFT and ab initio molecular dynamics simulations of possible nucleation processes on defect-laden graphene beginning with the AlCl precursor. Static calculations show that AlCl weakly physisorbs on perfect graphene, with binding energies less than 0.5 eV and very small barriers for diffusion along the surface. Covalent bonding is seen on graphene only at vacancy sites. Car-Parrinello molecular dynamics is used to study possible cluster nucleation mechanisms near characteristic vacancies. Simulations at 500 and 1000 K show that the AlCl is very reactive in the presence of the defect, quickly agglomerating and forming long AlCl chains with strong Al-Al bonds.

Sufian Alnemrat
Naval Postgraduate School

Date submitted: 30 Jan 2015 Electronic form version 1.4