Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Quantum Molecular Dynamics Validation of Nanocarbon Synthesis by High-Temperature Oxidation of Nanoparticles[1] CHUNYANG SHENG, KENICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, Collaboratory for Advanced Computing and Simulations, KOHEI SHIMAMURA, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, DEPARTMENT OF PHYSICS, KUMAMOTO UNIVERSITY COLLABORATION, CACS USC COLLABORATION — High-temperature oxidation of silicon-carbide nanoparticles (nSiC) underlies a wide range of technologies from high-power electronic switches for efficient electrical grid, thermal protection of space vehicles, to self-healing ceramic nanocomposites. Here, multimillion-atom reactive molecular dynamics simulations validated by *ab initio* quantum molecular dynamics simulations predict unexpected condensation of large graphene flakes during high-temperature oxidation of nSiC. In the validation process Small nSiC in oxygen environment is chosen to perform QMD simulation, then the QMD results provide the number of Si-O and C-O bonds as a function of time and high temperature, Same RMD simulation is simultaneously performed. We compare the time evolution of different bonds, and observe the condensation of large number of C-cluster nuclei into larger carbon clusters. We further provide the QMD simulation results as an input to a genetic algorithm, which trains the RMD force field parameters, the output force field produce results that are closer to the ground truth QMD simulation results.

[1]This research was supported by the Department of Energy (DOE)

Chunyang Sheng
Collaboratory for Advanced Computing and Simulations

Date submitted: 04 Nov 2015 Electronic form version 1.4