Formation of graphene flakes from oxidation of SiC nanoparticle
PANKAJ RAJAK, KENICHI NAMURA, RAJIV KALIA, AIICHIRO NAKANO, 
PRIYA VASHISHTA, Univ of Southern California — We have performed the largest 
(112 million atoms) reactive molecular dynamics simulation using reactive force fields 
to study the oxidation of a SiC nanoparticle on the full Blue Gene/P machine. The 
SiC nanoparticle of diameter 100 nm is surrounded by O$_2$ gas and heated to 2,800 K. Subsequently, we let the SiC nanoparticle oxidize at 2,800K. We observe formation 
of graphene-like flakes despite the harsh oxidation condition. We find the fractal 
dimension of the flakes is 1.85. We will discuss the implication of reaction kinetics 
on the structure and distribution of graphene flakes.