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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.

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