Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Anisotropic mechanical properties of hexagonal SiC sheet: a molecular dynamics study
MING YU, Univ of Louisville, EMILY LIU, duPont Manual High School, CONGYAN ZHANG, Univ of Louisville — The anisotropic mechanical properties of hexagonal SiC sheet have been studied using an efficient quantum mechanics molecular dynamics scheme based on a robust semi-empirical Hamiltonian (referred as SCED-LCAO) [PRB 74, 15540; PHYSE 42, 1]. It was found that the SiC sheet could sustain the heavy load up to about 20%. In particular, it was found that the SiC sheet also shows large difference in the strain direction. It will quickly crack after 20% of strain in armchair the direction, but it will be slowly destroyed after 30% in the zigzag direction, indicating the anisotropic nature of the mechanical properties of the SiC sheet. The nominal and 2D membrane stresses will be analyzed, from where we will obtain the 2D Young’s modulus at infinitesimal strain and the third-order (effective nonlinear) elastic modulus for the SiC sheet. The detail results and discussions will be reported in the presentation.

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Date submitted: 13 Nov 2014

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