Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

The Effect of Defects on Mechanical Properties and Failure Mechanisms of Graphene JONATHAN WILLMAN, JOSEPH GONZALEZ, University of South Florida, ROMAIN PERRIOT, Los Alamos National Laboratory, IVAN OLEYNIK, University of South Florida — Recent experiments involving nanoindentation of graphene have demonstrated counterintuitive increasing of Young's modulus with increasing concentrations of point defects in graphene. To fully resolve this controversy we perform large-scale molecular dynamics simulations of graphene nanoindentation. The relaible description of interatomic interactions is achieved by using recently developed screened environment-dependent bond order (SED-REBO) potential. The elastic properties of the defective graphene, the breaking strength and the mechanisms of fracture under indenter are investigated as a function of defect concentration and other factors specific to Atomic Force Microscopy (AFM) nanoindentation experiments.

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Date submitted: 06 Nov 2015 Electronic form version 1.4