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Mechanical Properties and Failure Mechanisms in Polycrystalline Graphene JOSEPH GONZALEZ, University of South Florida, ROMAIN PERRIOT, Los Alamos National Laboratory, IVAN OLEYNIK, University of South Florida — Large-scale growth of graphene using chemical vapor deposition produces polycrystalline material containing grain boundaries. Recent experiments demonstrate that polycrystalline graphene is nearly as strong as pristine. In this work, the mechanical properties of bi-crystal and polycrystalline graphene samples are investigated by simulating nano-indentation of a circular membrane using classical molecular dynamics and a novel Screened Environment Dependent Reactive Bond Order (SED-REBO) potential. The failure mechanisms and crack propagation in graphene samples containing grain boundaries are also discussed.

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