Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Phonon softening and mechanical failure of graphene under tensile strain JEONGWOON HWANG, JISOON IHM, Seoul Natl Univ, KYUNG-SUK KIM, MOON-HYUN CHA, Brown Univ — Phonon softening of graphene under tensile strain is investigated based on ab initio density functional theory calculations. From calculated phonon band structures, we show that the Kohn anomaly point shifts from a high symmetry K point to a lower symmetry one as a consequence of the Dirac point shift in the electronic band structure. We demonstrate that, over a wide range of tensile strain directions, the strain-induced enhancement of phonon softening can give rise to phonon instabilities resulting in a mechanical failure of graphene at lower strains. It is shown that there are two types of instabilities associated with phonons near K and Γ points, respectively, which induce symmetry-breaking structural distortions, and both of them lead to mechanical failure prior to the elastic failure commonly expected when the structural symmetry is retained.

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Date submitted: 05 Nov 2015 Electronic form version 1.4