Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Ideal Strength of graphene under general states of tensile strain[1]
MOON-HYUN CHA, Brown University, JEONGWOON HWANG, JISOON IHM, Seoul National University, KYUNG-SUK KIM, Brown Univ — Phonon softening of graphene under general directional tensile strain is investigated based on ab initio density functional theory calculations. Under a wide range of tensile strain configurations, we demonstrate that phonon instabilities are responsible for the mechanical failure of graphene through the strain-induced enhancement of phonon softening. It is shown that there are two types of phonon instabilities 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.

[1]This work was supported by the Korea Institute of Science and Technology (KIST) and Extreme Science and Engineering Discovery Environment (XSEDE).

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Date submitted: 15 Nov 2013 Electronic form version 1.4