Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Scattering of flexural acoustic phonons at graphene grain boundaries EDIT HELGEE, ANDREAS ISACSSON, Chalmers University of Technology — We have studied the scattering of long-wavelength flexural phonons against grain boundaries in graphene using molecular dynamics. The grain boundaries consist of arrays of dislocations, where the size of each dislocation is of the order of magnitude of the lattice constant. The small size of the dislocations suggests that long-wavelength phonons should be unaffected by the boundary. However, dislocations cause out-of-plane buckling of the graphene sheet. The width of the buckles can be on the order of nanometers, large enough to interact with long-wavelength vibrations. Of the two grain boundaries considered here, one shows no buckling while the other displays an out-of-plane buckling 0.5 nm high and approximately 1.5 nm wide. For the flat grain boundary, the phonon transmission approaches unity at long wavelengths. The buckled grain boundary, on the other hand, yields transmission coefficients between 0.4 and 0.6 for wavelengths exceeding 1 nm. Also, the flexural vibrations couple to longitudinal modes at the buckled grain boundary. This indicates that grain boundaries scatter long-wavelength flexural phonons, provided that the boundary causes out of plane buckling of the graphene sheet.

Edit Helgee
Chalmers University of Technology

Date submitted: 07 Nov 2013 Electronic form version 1.4