

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Long-wavelength vibrational modes in quasi-2D and tubular quasi-1D structures.¹ DAN LIU, DAVID TOMANEK, Michigan State University, ARTHUR G. EVERY, University of the Witwatersrand — We propose a continuum elasticity theory approach to predict long-wavelength vibrational modes of quasi-two-dimensional and quasi-one-dimensional tubular structures, such as empty and liquid-filled tubules, which are very hard to reproduce using the force-constant-matrix based atomistic approach based on *ab initio* calculation. We characterize the elastic behavior of these structures by a (3×3) elastic matrix characterizing a 2D membrane or a tubular wall, as well as the flexural rigidity of the membrane or the wall structure. We derive simple quantitative expressions for frequencies of long-wavelength acoustic modes, which we determine using 2D elastic constants calculated by *ab initio* density functional theory. Our results accurately reproduce observed and calculated long-wavelength phonon spectra of 2D graphene, 2D phosphorene, 1D microtubules of tubulin and 1D carbon nanotubes.

¹Supported by the NSF/AFOSR EFRI 2-DARE grant number #EFMA-1433459 and the African National Research Fundation.

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Date submitted: 15 Oct 2016

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