Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Influence of Misorientation on Graphene Moiré Patterns[1]
MARIE SMIRMAN, Oakland University, DOAA TAHA, Wayne State University, ARUNIMA SINGH, National Institute of Standards and Technology (NIST), ZHI-FENG HUANG, Wayne State University, KEN ELDER, Oakland University — In this work the influence of film-substrate misorientation on the strain-induced ordering of graphene films on various metallic surfaces is examined using a mesoscopic continuum model and first-principles atomistic calculations. The periodicity and free energy of the Moiré patterns that emerge are studied as a function of film-substrate adhesion strength for misfit strains far from and close to an incommensurate-commensurate phase transition. Interestingly the lowest energy states are found to be at small but finite misorientation even though these states have a higher domain wall density than the zero-misorientation states. First-principles density functional theory calculations are used to connect the results with experimental findings in graphene epitaxy. This combination of mesoscopic and atomistic approaches can be applied to the study of a wide range of strained 2D material systems including the III-Nitride monolayer systems.

[1]NSF Grant no. DMR-1506634

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Date submitted: 05 Nov 2016 Electronic form version 1.4