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Stacking 2D Materials: Bonding, Mechanics and Reconstructions

Ellad B. Tadmor

Professor Department of Aerospace Engineering and Mechanics, University of Minnesota, MN

ABSTRACT:

The synthesis of graphene, a one-atom thick two-dimensional (2D) graphitic sheet, was a revolution in materials physics. Since then a host of other 2D materials have been discovered that can be stacked to create layered heterostructures with remarkable properties (including the recent discovery of superconductivity in bilayer graphene). Due to the weak van der Waals interaction between layers, the resulting structures can be incommensurate and therefore challenging to model. First, high-quality interatomic potentials are required. We describe recent work to develop traditional physics-based and new machine learning potentials for 2D heterostructures. Second, in order to simulate the mechanics of large-scale 2D heterostructures we developed a hybrid continuum-atomistic computational framework based on the subdivision finite element method. Simulations of twisted graphene bilayers show a transformation from an initially incommensurate structure to nearly commensurate structures separated by localized solitons. The mechanism for this transformation is discussed as well as an interesting scaling behavior related to the initial imposed twist, which creates a qualitative change in electron diffraction patterns subsequently verified experimentally.

BIOGRAPHY:

Ellad B. Tadmor is a Professor of Aerospace Engineering and Mechanics at the University of Minnesota (USA). He received his B.Sc. and M.Sc. in Mechanical Engineering from the Technion -- Israel Institute of Technology in 1987 and 1991, and his Ph.D. from Brown University (USA) in 1996. His research focuses on the development of multiscale theories and computational methods for predicting the behavior of materials directly from the interactions of the atoms making up the material. He has published over 60 papers in this area and two textbooks (see http://modelingmaterials.org). Prof. Tadmor is the Director of the Knowledgebase of Interatomic Models (OpenKIM.org) project which is tasked with developing standards for atomistic simulations and improving transferability of interatomic potentials. He was a Postdoctoral Research Fellow at Harvard University (USA), Associate Professor at the Technion (Israel), and Erasmus Mundus Scholar at the Ecole Normale Superieure in Lyon (France). He received the MRS Graduate Student Award in 1995 for his work on developing the quasicontinuum method, one of the leading multiscale methods, as well as numerous awards for excellence in teaching including the Salomon Simon Mani Award in 2001. Prof. Tadmor is on the Editorial Board of the Journal of Elasticity.