

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Mechanical Behavior of Graphene Nanomeshes MENGXI CHEN, LIN HU, ASHWIN RAMASUBRAMANIAM, DIMITRIOS MAROUDAS, Univ of Mass - Amherst — Graphene nanomeshes (GNMs) are ordered, defect-engineered graphene nanostructures consisting of periodic arrays of nanopores in the graphene lattice with neck widths less than 10 nm. The electronic, transport, and mechanical properties of GNMs can be tuned by varying the structural, chemical, and architectural parameters of the nanomeshes, namely, their porosity, as well their pore lattice structure, pore morphology, and pore edge passivation. Here, we study the mechanical response of GNMs to uniaxial tensile straining and determine their mechanical properties based on molecular-dynamics simulations of dynamic deformation tests according to a reliable bond-order interatomic potential. We establish the dependences of the elastic modulus, fracture strain, ultimate tensile strength, and toughness on the nanomesh porosity and derive scaling laws for GNM modulus-density and strength-density relations. We also establish the dependence of the above properties on pore morphology, for GNMs with circular and elliptical pores over a range of aspect ratios, and on pore edge hydrogen passivation that causes elastic stiffening and strength reduction. The underlying mechanisms of crack initiation and propagation and nanomesh failure also are characterized.

Mengxi Chen
Univ of Mass - Amherst

Date submitted: 05 Nov 2015

Electronic form version 1.4