Contribution ID : **159** Type : **Poster**

BN-Defect Engineering in TPH-Graphene Mechanics

Tetra penta hepta graphene (TPH-gr) is a non hexagonal two dimensional carbon allotrope whose 4, 5, and 7 membered ring network can generate strong elastic anisotropy and unconventional fracture pathways. We conduct molecular dynamics simulations of pristine TPH-gr and structures containing substitutional boron nitrogen (BN) pair defects, using the Tersoff potential. Direction dependent elastic modulus and ultimate tensile strength are extracted from uniaxial tension tests over T = 100 to 700 K, and the deformation and failure mechanisms are analyzed via atomistic stress maps and bond topology tracking. Pristine TPH-gr exhibits pronounced anisotropy governed by stress focusing at specific ring junctions that act as crack nucleation sites. Introducing BN pairs reduces the Young's modulus for tension along the x direction, indicating defect induced softening under this loading orientation. Raising temperature further decreases the modulus in all cases, consistent with enhanced thermal bond fluctuations and earlier strain localization. Overall, BN pair incorporation provides a route to defect engineer the stiffness and failure behavior of TPH-gr for robust 2D nanoarchitectures.

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Session Classification : Poster Fisica del Estado Solido