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Mechanical Behavior of Nanocomposite Structures from Interlayer Bonding in Twisted Bilayer Graphene MENGXI CHEN, University of Massachusetts, Amherst, ANDRE MUNIZ, Federal University of Rio Grande do Sul, Porto Alegre, Brazil, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We report a systematic computational analysis of the mechanical behavior of graphene-diamond nanocomposites formed through interlayer covalent bonding of twisted bilayer graphene with commensurate bilayers. The interlayer bonding is induced by patterned hydrogenation that leads to formation of superlattices of 2D nanodiamond domains embedded between the two graphene layers with the periodicity of the underlying Moiré pattern. The analysis is based on molecular-dynamics (MD) simulations of uniaxial tensile straining tests according to a reliable interatomic bond-order potential. The mechanical response of the nanocomposites is explored as a function of their structural parameters, which include the bilayer's twist angle, the stacking type of the nanodomains where the interlayer bonds are formed, the interlayer bond density, and the concentration of sp^3-bonded C atoms. We determine the mechanical properties of these 2D materials and identify a range of structural parameters over which their fracture is ductile, mediated by void formation and growth, in contrast to the typical brittle fracture of graphene. We analyze the ductile fracture mechanisms and systematically probe the brittle-to-ductile transition.

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