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Electronic and Mechanical Properties of Hydrogenated Irradiated and Amorphous Graphene ASANKA WEERASINGHE, Department of Physics, University of Massachusetts - Amherst, ASHWIN RAMASUBRAMANIAM, Department of Mechanical and Industrial Engineering, University of Massachusetts - Amherst, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts - Amherst — Defect engineering and chemical functionalization of graphene are promising routes for fabrication of carbon nanostructures and 2D metamaterials with unique properties and function. Here, we use hydrogenation of irradiated, including irradiation-induced amorphous, graphene as a means of studying chemical functionalization effects on its electronic structure and mechanical response. We use molecular-dynamics simulations based on a reliable bond-order potential to prepare the hydrogenated configurations and carry out dynamic deformation tests at constant strain rate and temperature. Our mechanical tests show that hydrogenation does not affect the ultimate tensile strength (UTS) of the irradiated graphene sheet if the hydrogenated C atoms remain sp^2-hybridized; however, upon inducing sp^3 hybridization of these C atoms, UTS decreases by about 10 GPa. Furthermore, the fracture strain of the irradiated structure decreases by up to 30% upon hydrogenation independent of the hybridization type. We also report results for the electronic structure of hydrogenated configurations based on a density-functional tight-binding approach and assess the potential for tuning the electronic properties of these defective, functionalized graphenes.

Asanka Weerasinghe
Univ of Mass - Amherst

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