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Defect-induced amorphization of single-layer graphene: structure and mechanical properties CORINNE CARPENTER, ASHWIN RAMASUBRAMANIAM, DIMITRIOS MAROUDAS, University of Massachusetts Amherst —
Defect engineering of graphene provides a potential route for tuning its mechanical, electronic, and chemical properties. While individual defects in single-layer graphene have been investigated in much detail, collective interactions of multiple defects are less well understood. In this work, we address the effects of introducing populations of vacancies in single-layer graphene using classical molecular-dynamics simulations based on reliable bond-order potentials. We study random distributions of vacancies in a single graphene layer with vacancy concentration and temperature being the key parameters in the analysis. We demonstrate that a crystalline-to-amorphous structural transition occurs at vacancy concentrations of 5-10% leading to complete loss of long-range order in the graphene layer. We conduct a systematic parametric study of this phenomenon accompanied by a detailed structural analysis of the defective sheets. We also present systematic studies of tensile tests on these defective graphene sheets and identify trends for the ultimate tensile strength, failure strength, and toughness as a function of vacancy concentration. The implications of our findings for tuning the mechanical and electronic properties of single-layer graphene are discussed.

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