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Vacancy-induced order-to-disorder transition in single-layer graphene CORINNE CARPENTER, ASHWIN RAMASUBRAMANIAM, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — Defect engineering provides a potential route for tuning the mechanical, electronic, and chemical properties of graphene. While individual defects in single-layer graphene have been investigated in much detail, the outcomes of collective interactions of multiple defects remain elusive. In this work, we address the collective interaction of populations of vacancies in single-layer graphene using classical molecular-dynamics simulations based on reliable bond-order potentials; we examine random vacancy distributions with the vacancy concentration and temperature being the key parameters in the analysis. We demonstrate that a crystalline-to-amorphous structural transition occurs as the vacancy concentration in single-layer graphene increases beyond a critical level; the transition leads to complete loss of long-range order in the graphene layer. The onset of this order-to-disorder transition typically occurs over the vacancy concentration range from 10 to 20% and is independent of the details of the interatomic interactions in the classical potentials employed. We present a systematic parametric study of the phenomenon and discuss the implications of our findings for the mechanical and electronic properties of single-layer graphene.

Ashwin Ramasubramaniam
University of Massachusetts Amherst

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