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Coordination Defects: a Novel Type of Grain Boundary-Producing Defect BENJAMIN KATZ, VINCENT CRESPI, Pennsylvania State University — A novel defect type in two-dimensional systems is presented, which involves the local coordination number of atoms in an otherwise regular structure. While point-like by itself, such a 'coordination defect' is shown to have a dramatic influence on the growth of the system following its formation due to its introduction of a mismatch in bond network topology and physical ring size. This defect can be of varying size, producing predictable changes in the growth of the system after its appearance. The potential growth pathways of an example graphene system are followed after the occurrence of such a defect using molecular dynamics and first-principles calculations; the inherent tension between the topological requirements and the actual chemical/physical structure that occurs as the system heals the defect can result in varied new morphologies, including a runaway feedback resulting in the spawning of one or more flat finite grain boundaries. Energy comparisons from first principles are used to evaluate the likelihood of this result under various conditions. The appearance of this defect type is predicted to have similar ramifications across a broad array of two-dimensional systems, potentially providing a new method of controlling grain boundary behavior and location.

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