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Grain boundary properties and collective dynamics of inversion domains in binary two-dimensional materials DOAA TAHA, Department of Physics and Astronomy, Wayne State University, SIMISO MKHONTA, Department of Physics, University of Swaziland, KEN ELDER, Department of Physics, Oakland University, ZHI-FENG HUANG, Department of Physics and Astronomy, Wayne State University — Grain boundary structures and dynamics of binary two-dimensional materials are investigated through the development of a phase field crystal model. The model is parameterized for the study of hexagonal boron nitride monolayers, to identify the angle dependence of grain boundary energy and defect structures for both symmetric and asymmetric tilt boundaries. Our results not only reproduce all types of dislocation cores observed in previous experiments and first-principles calculations, but also predict some new defect structures for various grain boundary misorientations, particularly the 60-degree inversion domains. In addition, we identify a new mechanism of grain coarsening dynamics, as originated from the impinging of 60-degree misoriented grains and the subsequent formation of triangle or truncated-triangle shaped domains that are separated from the surrounding matrix via inversion domain boundaries. The domain evolution and shrinking processes are governed by the collective atomic displacement of the connected square-octagon (4|8) pairs along the boundary lines and the heart-shaped defects at the junctions. This defect-mediated collective dynamics of inversion domains is important for understanding the complex mechanisms of grain growth in binary 2D materials.

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