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Structural and transport properties of finite length grain boundaries in two-dimensional materials YUANXI WANG, VINCENT CRESPI, Pennsylvania State University — Grain boundaries in two dimensional materials such as graphene and monolayer transition metal dichalcogenides are unfortunate consequences of grains growing in different orientations, keeping the material away from a monocrystalline ground state. We show that when 2D materials are grown on substrates with gaussian curvatures, grain boundaries produced from self-intersections are in fact the ground state. They screen out the curvature imposed by the substrate and form finite length chain structures, terminating with cone and saddle shapes of partial disinclinations. The structural stability and transport properties of finite length grain boundaries are studied at the tight-binding level. Every dislocation in the grain boundary contributes an intrinsic pseudo-flux and induces loop currents during transport. We further show that transport properties depend sensitively on the number of dislocations in the grain boundary.

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