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Mechanisms of Bowtie- and Star-Shaped MX_2 Nanoisland Formation VASILII I. ARTYUKHOV, ZHILI HU, ZHUHUA ZHANG, BORIS I. YAKOBSON, Rice University — A large number of experimental studies over the last few years observed the formation of unusual highly symmetric polycrystalline twinned nanoislands of transition metal dichalcogenides, resembling bowties or stars. Here we analyze their morphology in terms of equilibrium and growth shapes. We propose a mechanism for their formation via collision of concurrently growing islands and validate the theory with phase-field simulations. Finally, we use first-principles calculations to propose an explanation of the predominance of high-symmetry polycrystals with 60-degree lattice misorientation angles.

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