Three-dimensional dislocation networks in α-Iron twist grain boundaries: Insights from first-principles neural network interatomic potentials

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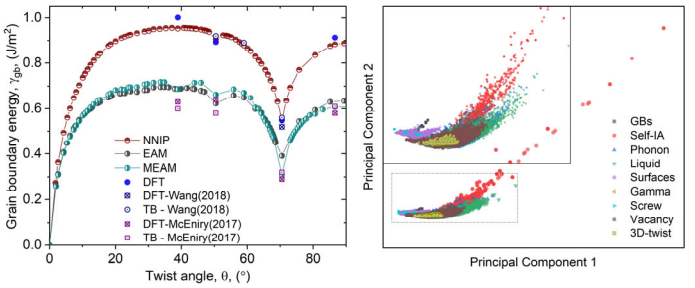
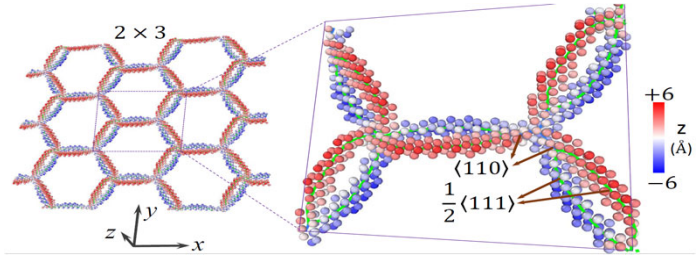
Purpose: Uncover the relationship between the structural and energy of twist grain boundaries(TWGBs) in α-Iron.

Outline: The atomic structure and formation energy of TWGBs were investigated using molecular statics in conjunction with neural network interatomic potentials(NNIPs).

Result: We charted the grain boundary energy of TWGBs for (100), (110), and (111) terminations, achieving concordance between NNIP predictions and DFT calculations. Exploring dislocation networks in TWGBs with small twist angles unrevealed distinct network patterns. Squared and hexagonal dislocation networks patterns in (100) and (110) TWGBs were obtained, mirroring experimental observations in BCC metals.

Significantly, (111) TWGBs with small twist angles exhibited a novel 3D dislocation pattern, a phenomenon uncovered for the first time. The novel 3D dislocation pattern was validated through principal component analysis, NNIP ensemble model, and further crossing verification using other independent machine learning potentials. Our work sheds light on the uncharted territories of dislocation networks in certain configurations.





Computing system:	SQUID General Purpose CPU nodes
node-hour	20,500 node-hour
memory used	256 GB
parallelize	4 nodes