Supporting Information

Mechanically-Driven Grain Boundary Formation in Nickel Nanowires

Lihua Wang,[†,‡] Deli Kong,[†] Yin Zhang,[§] Lirong Xiao,[†] Yan Lu,[†] Zhigang Chen,[‡] Ze Zhang,[⊥†] Jin Zou,[‡,//] Ting Zhu,[3*§] and Xiaodong Han[1*†]*

[†]Beijing Key Lab of Microstructure and Property of Advanced Material, Institute of Microstructure and Properties of Advanced Materials, Beijing University of Technology, Beijing, 100124, China

[‡]Materials Engineering; The University of Queensland, Brisbane, QLD 4072, Australia

[†]Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

[⊥]Department of Materials Science, Zhejiang University, Hangzhou, 310008, China

[//]Centre for Microscopy and Microanalysis, The University of Queensland, Brisbane, QLD 4072, Australia

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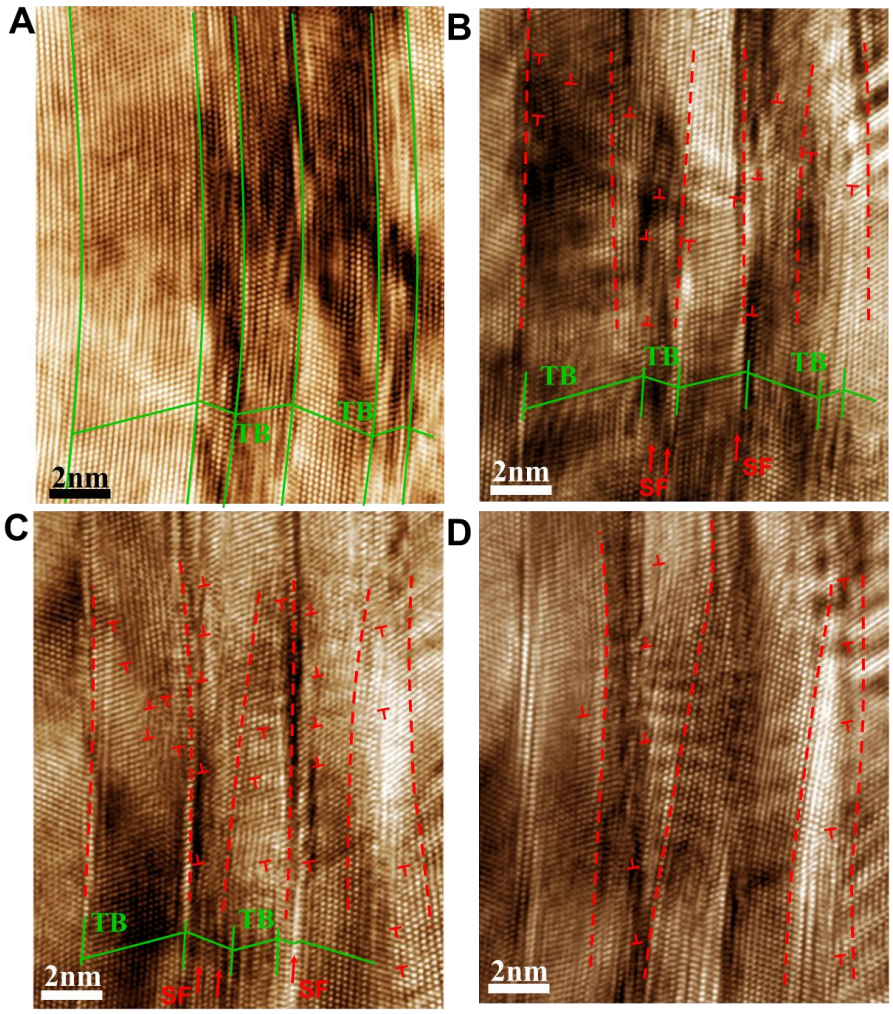

Fig. S1. *In situ* atomic-scale observation of dislocations at and near twin boundaries (TBs) formed during plastic bending of a nanotwinned Ni nanowire. (A) A typical HRTEM image captured under a low bending load. Few dislocations were observed. Curved TBs and lattice planes are highlighted by the dotted green lines. (B) Further bending resulted in the accumulation of many full dislocations (marked by the symbol of ⊥) randomly distributed in twin lamellae. (C) An increasing amount of dislocations accumulated in twin lamellae. Some dislocations aggregated to form a dislocation array regularly arranged one above another. (D) Two arrays of dislocations with opposite Burgers vectors, each forming a low-angle GB. The two dislocation arrays created two wedge-shaped regions, indicating the formation of disclination dipoles. A similar configuration was experimentally observed in nanocrystalline Fe with a body-centred cubic structure.

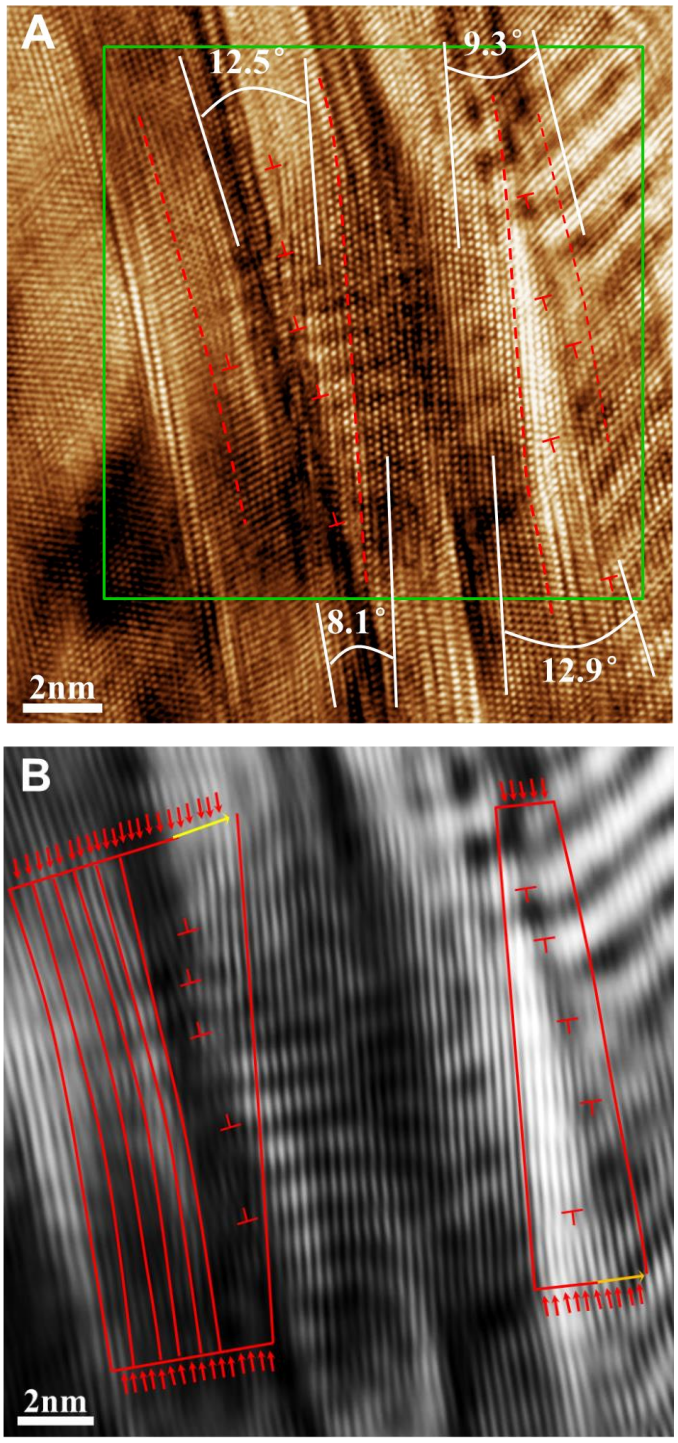

Fig. S2. The disclination dipoles subdividing the NWs into a 6 nm×11 nm sized sub-grain with a GB angle of ~10°. (A) Two arrays of dislocations formed the disclination dipoles, subdividing the NWs into a 6 nm×11 nm sized sub-grain with a GB angle of ~10°. (B) {111} lattice fringes obtained by HRTEM image filtering, showing the two dislocation arrays more clearly.

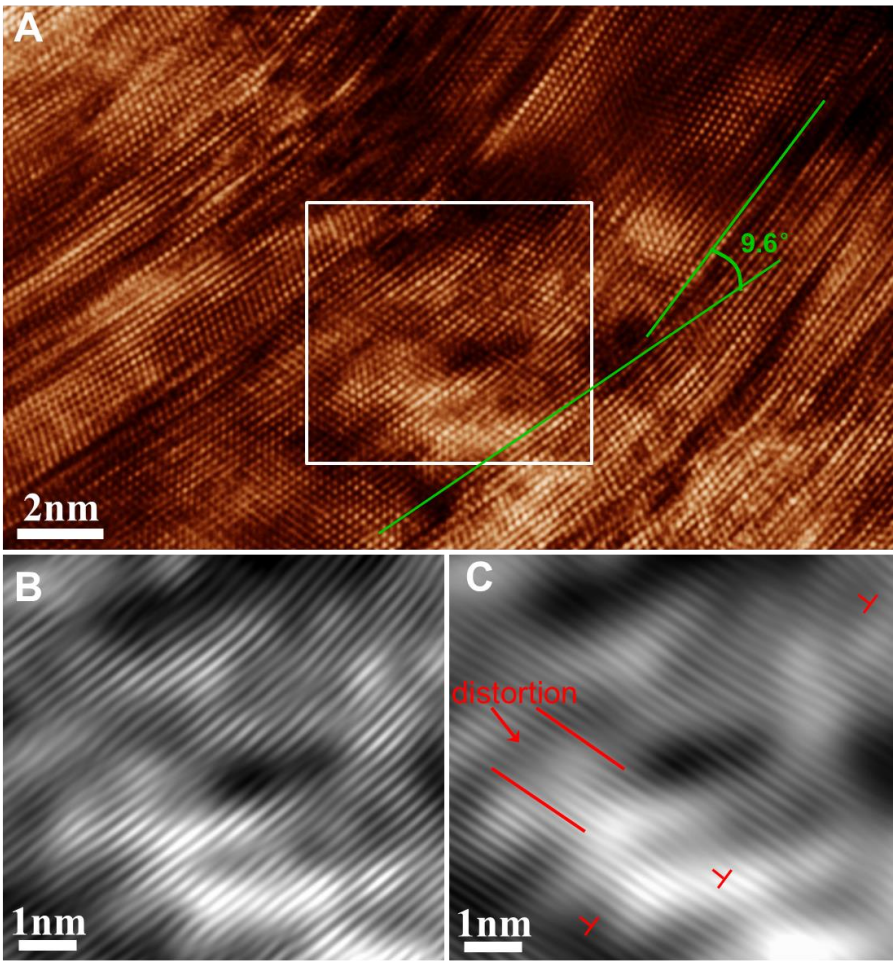

Fig. S3. Two sets of {111} lattice fringes obtained by filtering of HRTEM images, showing that no dislocation arrays were observed when the lattice misorientation across the incipient GB was ~9.6°. (A) Localized plastic bending deformation was accommodated by the curved lattice and TBs, when the lattice misorientation across the incipient GB was ~9.6°. (B, C) Two sets of {111} lattice fringes obtained by filtering of HRTEM images; no dislocation arrays were observed.

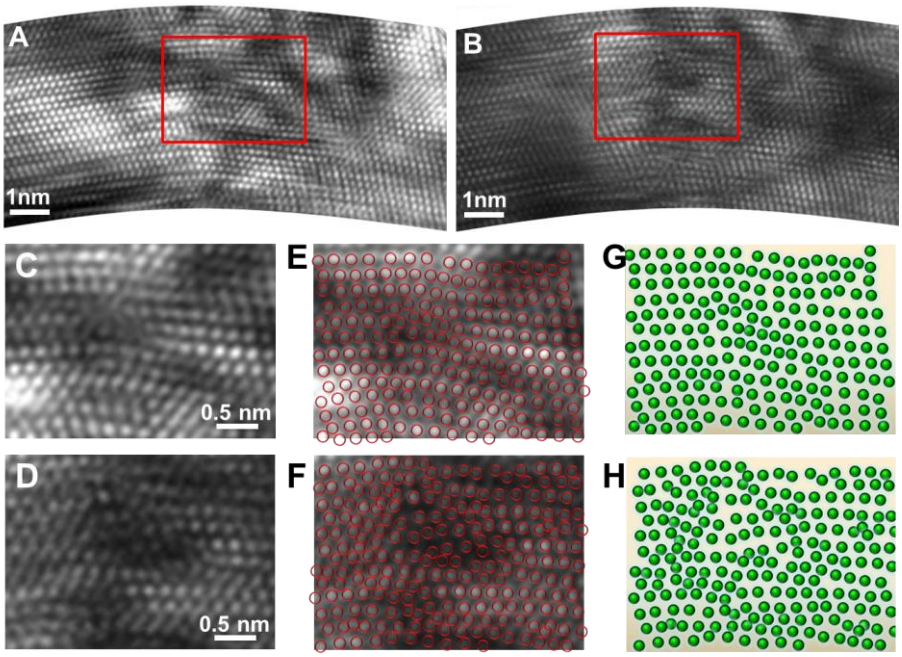

Fig. S4. *In situ* observation showing that the original parallelogram-shaped lattice became irregular and no regularly arranged dislocation arrays can be identified in the GB region. (A) HRTEM image corresponding to Fig. 3C in the paper, showing a high density of dislocations in the plastically bent lattice. (B) HRTEM image corresponding to Fig. 3D in the paper. (C, D) Enlarged HRTEM images taken from the red framed region of (A) and (B), respectively. (E, F) Atoms identified in (C, D) are drawn as circles that are superimposed on the corresponding HRTEM image. (G, H) Atoms identified in (C, D) are drawn separately, showing that the original parallelogram shaped lattice became irregular and no regularly-arranged dislocation arrays can be identified in the GB region.

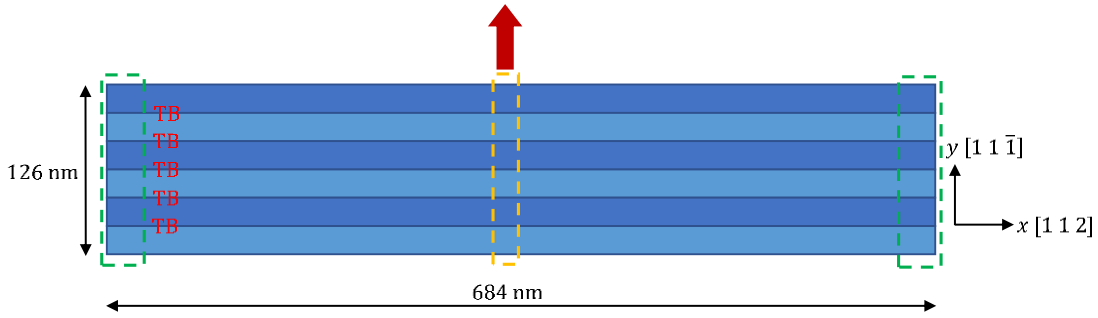

Fig. S5. Schematic illustration of molecular dynamics simulation of plastic bending of a nanotwinned Ni NW. The orange boxed region is moved upward (as indicated by the arrow) while the green boxed regions are fixed, so as to mimic a three-point bending process. Such a loading scheme of three-point bending facilitates the generation of a plastic hinge in the simulated NW, thereby resulting in a symmetric tilt GB similar to the bending-induced GBs observed in experiment.

Supplementary Movie S1: Molecular dynamics simulations of plastic bending of a nanotwinned Ni nanowire, resulting in the formation of in a nearly symmetric tilt GB similar to the bending-induced GBs observed during *in situ* TEM experiments.