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Twin and dislocation mechanisms in tensile W single crystal with temperature change: A molecular dynamics study Supplementary Materials

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1. Model parameters

Supplementary Table 1: Parameters of the present potential, in comparison with those form experiment, density-functional theory (DFT) calculations, the modified embedded atom method (MEAM) potential and the bond-order potential (BOP). a: the lattice constant (Å); E_c: cohesive energy (eV/atom); E_f: formation energy (eV); v: vacancy: SIA: self-interstitial atom; tet: tetrahedral interstitial; oct: octahedral interstitial; $db\langle ijk\rangle$: $\langle ijk\rangle$ dumbbell interstitial configuration.

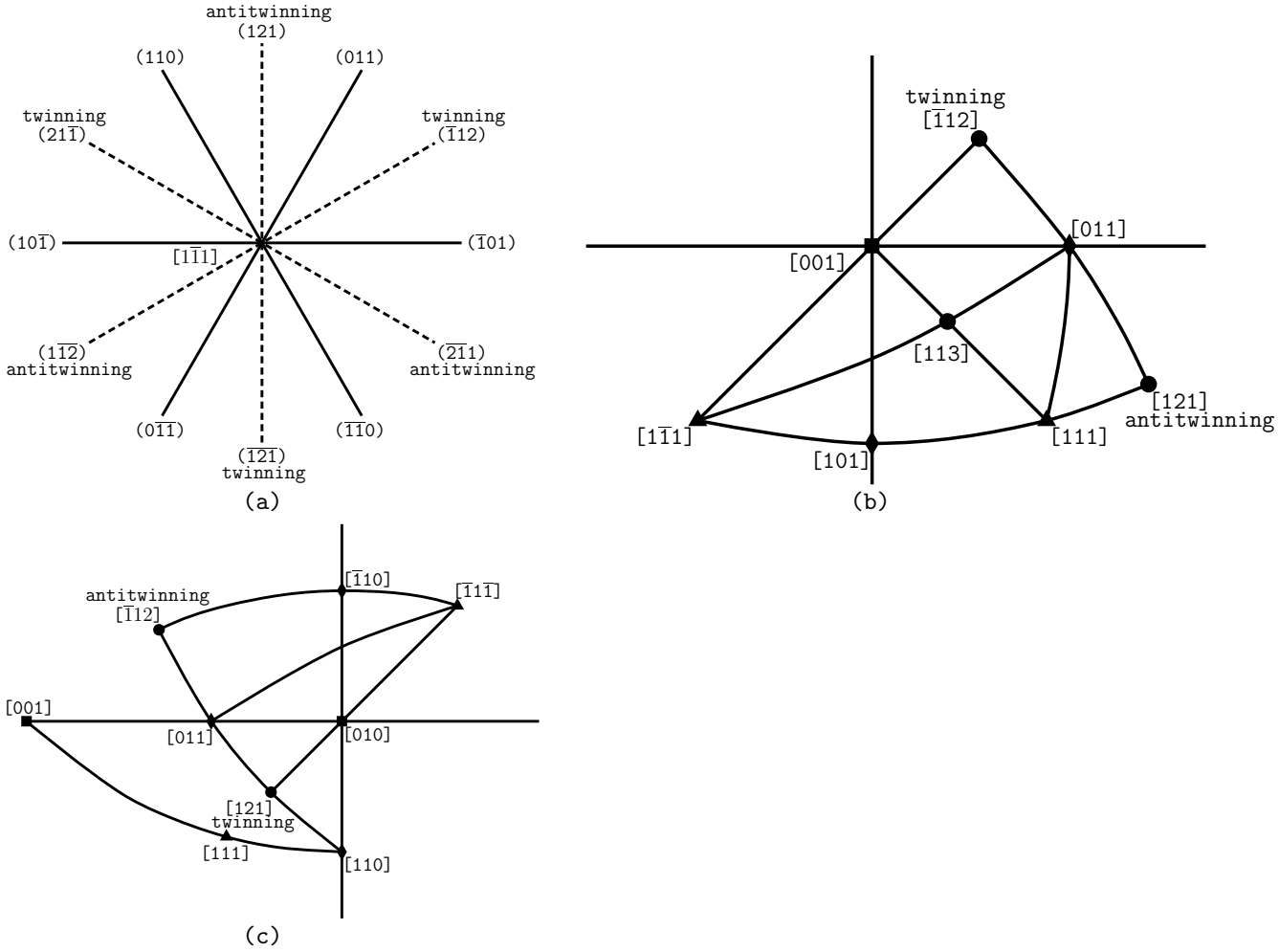
	present	DFT	Experimental	BOP	MEAM[k]
a	3.165	3.18[c]	3.165[d]	3.165[h,i]	3.164
E_c	-8.90	-7.406[i]	-8.90[e]	-8.906[h], -8.89[i]	-8.66
$E_{f,v}$	3.63	3.46[a], 3.56[b]	3.7 ± 0.2[f]	3.52[h], 1.68[i]	3.95
$E^{SIA}_{f,tet}$	10.31	11.64[a], 11.05[b]		10.75[h]	
$E^{SIA}_{f,oct}$	10.41	11.99[a], 11.68[b]		12.05[h]	
$E^{SIA}_{f,db\langle 100\rangle}$	10.29	11.74[a], 11.49[b]		12.01[h]	
$E^{SIA}_{f,db\langle 110\rangle}$	10.18	10.10[a], 9.84[b]		9.53[h]	8.98
$E^{SIA}_{f,db\langle 111\rangle}$	9.51	9.82[a], 9.55[b]	9.06 ± 0.63[g]	9.33[h]	

a Ref.[1]
b Ref.[2]
c Ref.[3]
d Ref.[4]
e Ref.[5]
f Ref.[6]
g Ref.[7]
h Ref.[8]
i Ref.[9]
k Ref.[10]

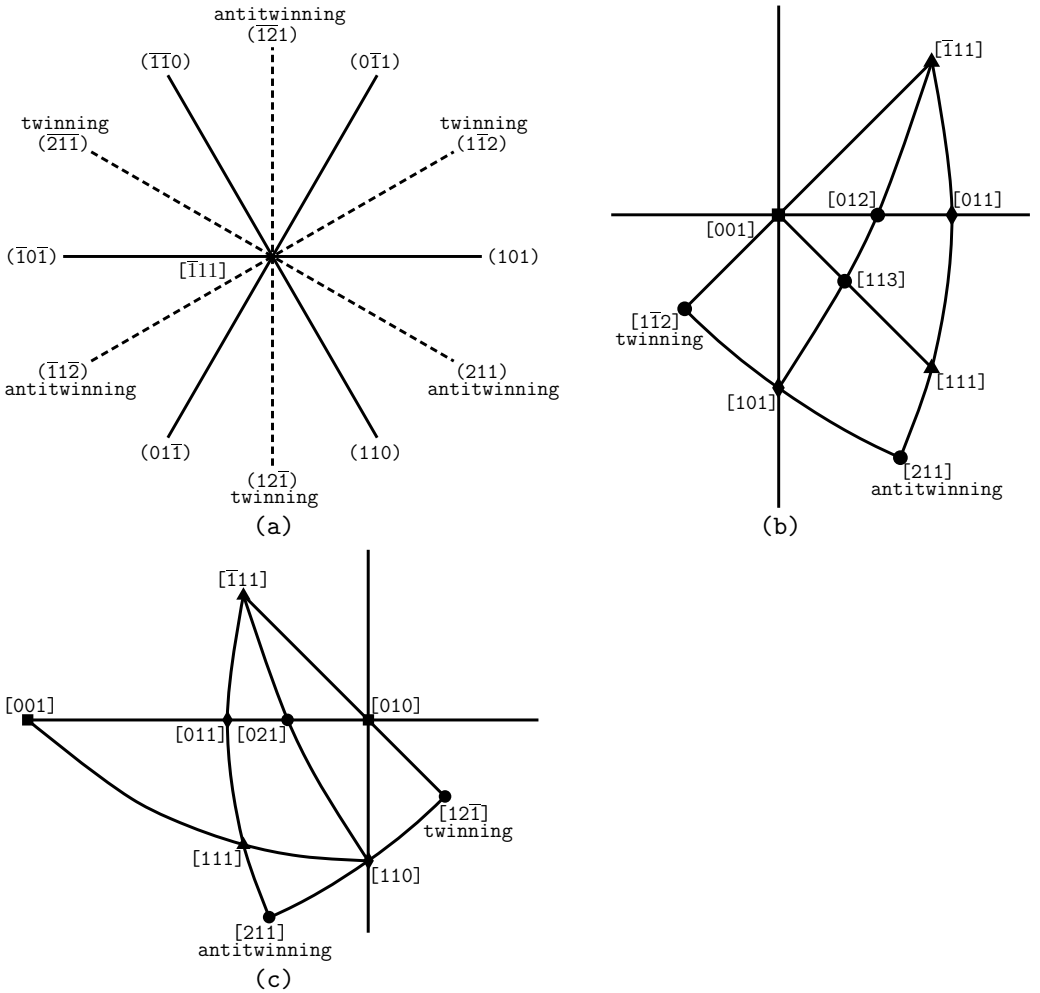
Supplementary Table 2: Model parameters: angle from [001] (°), directions, dimensions (nm) and the number of W atoms.

Angle from [001]	x	y	z (tensile direction)	Dimensions ($x \times y \times z$)	No. of W atoms
0	100	010	001	$12.7 \times 12.7 \times 12.7$	128,000
5.1	$1\bar{1}0$	$88\bar{1}$	1,1,16	$9.0 \times 14.4 \times 15.2$	123,840
10.0	$1\bar{1}0$	$44\bar{1}$	118	$9.0 \times 10.9 \times 15.4$	95,040
15.8	$1\bar{1}0$	$55\bar{2}$	115	$9.0 \times 11.6 \times 16.4$	108,000
19.5	$1\bar{1}0$	$22\bar{1}$	114	$9.0 \times 11.4 \times 16.1$	103,680
25.2	$1\bar{1}0$	$33\bar{2}$	113	$9.0 \times 11.9 \times 16.8$	112,640
29.5	$1\bar{1}0$	$55\bar{4}$	225	$9.0 \times 12.9 \times 18.2$	132,000
35.3	$1\bar{1}0$	$11\bar{1}$	112	$9.0 \times 11.0 \times 15.5$	96,000
40.3	$1\bar{1}0$	$55\bar{6}$	335	$9.0 \times 11.7 \times 16.6$	110,080
46.7	$1\bar{1}0$	$22\bar{3}$	334	$9.0 \times 13.1 \times 18.5$	126,000
50.5	$1\bar{1}0$	$7, 7, \overline{12}$	667	$9.0 \times 14.8 \times 13.9$	116,160
54.7	$1\bar{1}0$	$11\bar{2}$	111	$9.0 \times 15.5 \times 11.0$	96,000
60.5	$1\bar{1}0$	$22\bar{5}$	554	$9.0 \times 10.9 \times 15.4$	95,040
64.8	$1\bar{1}0$	$11\bar{3}$	332	$9.0 \times 12.6 \times 17.8$	126,720
70.5	$1\bar{1}0$	$11\bar{4}$	221	$9.0 \times 13.4 \times 19.0$	144,000
76.7	$1\bar{1}0$	$11\bar{6}$	331	$9.0 \times 11.7 \times 16.6$	109,440
82.0	$1\bar{1}0$	$1, 1, \overline{10}$	551	$9.0 \times 16.0 \times 11.3$	102,000
86.3	$1\bar{1}0$	$1, 1, \overline{22}$	11,11,1	$9.0 \times 14.0 \times 14.8$	116,640
90	$\bar{1}10$	001	110	$13.4 \times 9.5 \times 13.4$	108,000
5.7	100	$0, 10, \bar{1}$	0,1,10	$9.5 \times 12.7 \times 12.7$	96,960
11.3	100	$05\bar{1}$	015	$9.5 \times 12.9 \times 12.9$	99,840
15.9	100	$07\bar{2}$	027	$9.5 \times 13.8 \times 13.8$	114,480
21.8	100	$05\bar{2}$	025	$9.5 \times 13.6 \times 13.6$	111,360
26.6	100	$02\bar{1}$	012	$9.5 \times 14.2 \times 14.2$	120,000
31.0	100	$05\bar{3}$	035	$9.5 \times 12.9 \times 12.9$	99,960
36.9	100	$04\bar{3}$	034	$9.5 \times 12.7 \times 12.7$	96,000
40.6	100	$07\bar{6}$	067	$9.5 \times 14.6 \times 14.6$	127,500
45	100	$01\bar{1}$	011	$9.5 \times 9.0 \times 9.0$	48,000
Additional orientations	$1\bar{1}2$	$7\overline{14}$	131	$11.6 \times 12.9 \times 15.7$	148,500
	$\bar{1}01$	$1\bar{1}1$	121	$9.0 \times 11.0 \times 15.5$	96,000
	$11\bar{2}$	$\overline{13}, 5, \overline{4}$	153	$11.6 \times 9.2 \times 18.7$	126,000
	$1\bar{1}2$	$11, \bar{5}, \bar{8}$	351	$11.6 \times 9.2 \times 18.7$	126,000
	$12\bar{3}$	$\overline{41}, 16, \bar{3}$	397	$11.8 \times 14.0 \times 14.9$	155,680
	$12\bar{3}$	$\bar{2}10$	365	$11.8 \times 10.6 \times 13.2$	105,000
	$10\bar{2}$	$\bar{2}2\bar{1}$	452	$8.5 \times 11.4 \times 17.0$	103,680
	$01\bar{3}$	$\bar{4}31$	562	$10.0 \times 12.9 \times 12.8$	104,000

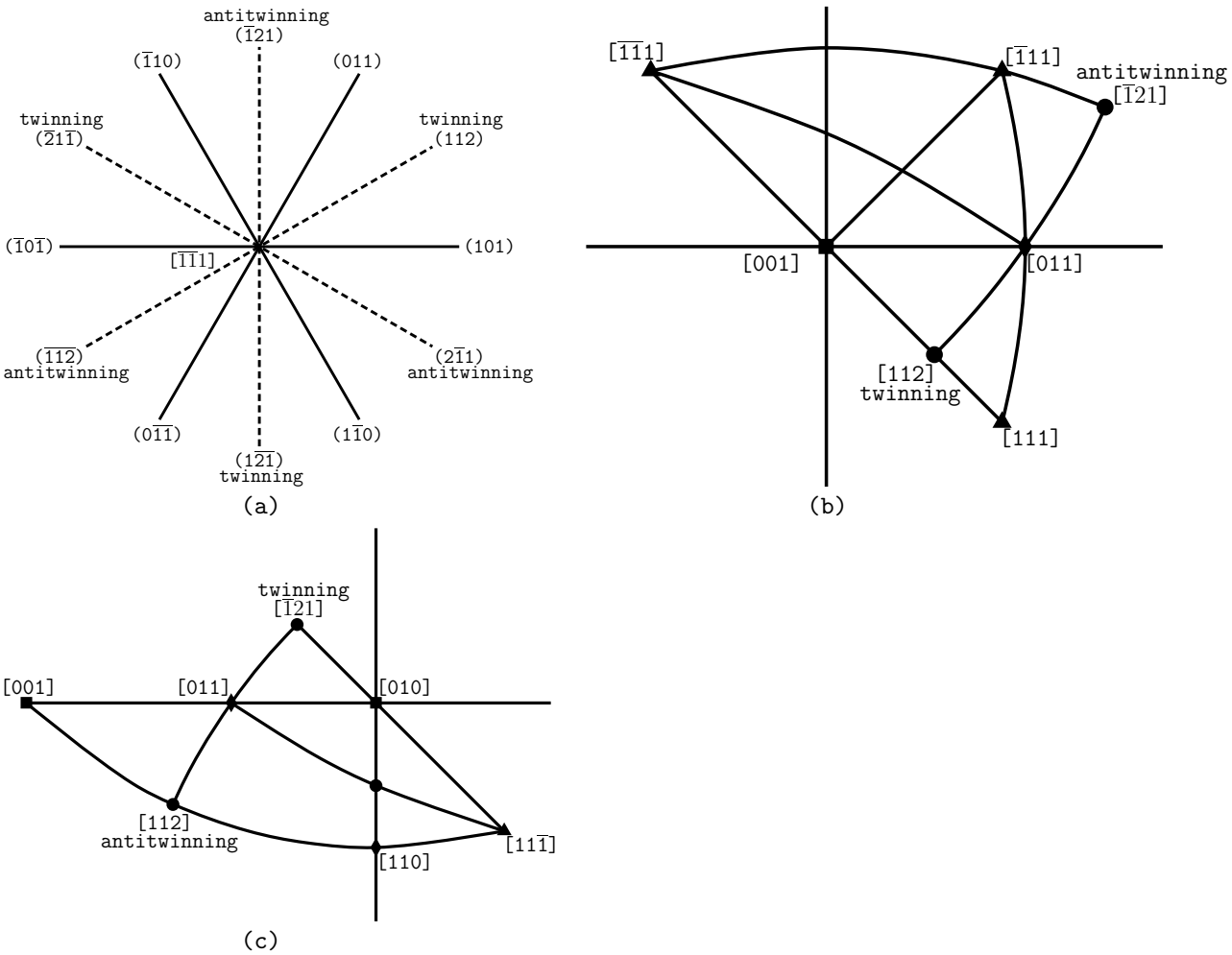
2. Orientation divisions according to $[1\bar{1}1]$, $[\bar{1}11]$ and $[\overline{1}\overline{1}1]$ slip directions



Supplementary Figure 1: (Color online) (a) Schematic figure showing the twinning and antitwinning planes along the $[1\bar{1}1]$ slip direction;(b-c) Standard [001] and [010] stereographic projections for cubic crystals illustrating orientation division according to the $[1\bar{1}1]$ slip direction within the standard stereographic triangle.

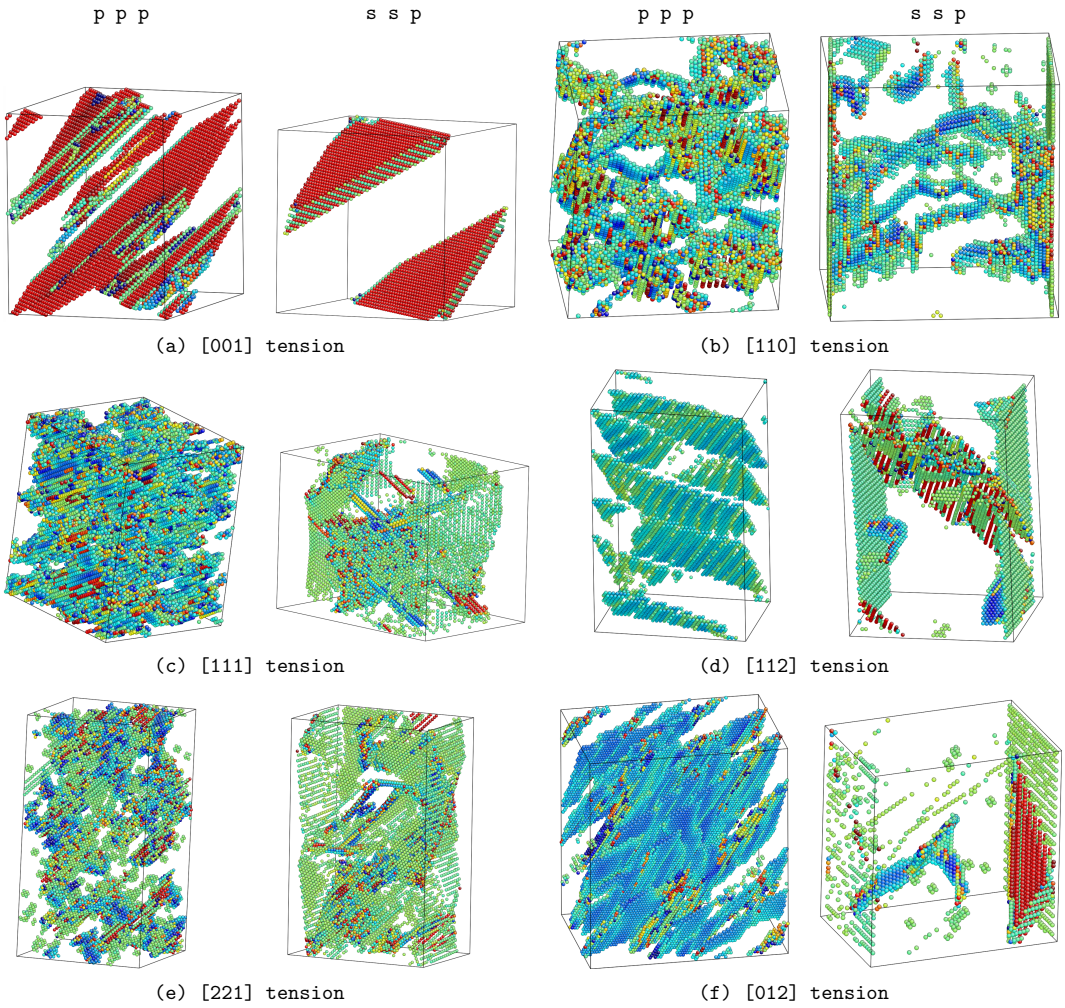


Supplementary Figure 2: (Color online) (a) Schematic figure showing the twinning and antitwinning planes along the $[\bar{1}11]$ slip direction. (b-c) Standard [001] and [010] stereographic projections for cubic crystals illustrating orientation division according to the $[\bar{1}11]$ slip direction within the standard stereographic triangle.



Supplementary Figure 3: (Color online) (a) Schematic figure showing the twinning and antitwinning planes along the $[\overline{1}\overline{1}1]$ slip direction. (b-c) Standard [001] and [010] stereographic projections for cubic crystals illustrating orientation division according to the $[\overline{1}\overline{1}1]$ slip direction within the standard stereographic triangle.

3. Influence of different boundary conditions on the deformation mechanism of single crystal W



Supplementary Figure 4: (Color online) Yield behaviors of bulk materials and nanowires with orientations of [001], [110], [111], [112], [221] and [012] at 10K. The atoms are coloured according to the centro-symmetry parameter (CSP)

To investigate the influence of different boundary conditions on the deformation mechanism of single crystal W, tensile tests on nanowires (boundary conditions: s s p along x y z) with orientations of [001], [110], [111], [112], [221] and [012] are simulated at 10 K and compared with their bulk counterparts. As shown in Supplementary Fig.4, it is found that the nanowire with [001] orientation yields by twinning, while the nanowires with orientations of [110], [111] and [221] yield by dislocation slip, which are consistent with their bulk counterparts (Supplementary Fig.4a-c and e). As for [112] and [012] orientations (Supplementary Fig.4d and f), they initially yield by unstable stable twin embryos and further deform through dislocation slip for bulk materials (like Fig.12a-b), while yield by both twin

deformation and minor dislocation activities for nanowires (like Fig.12c-d), which all belong to the intermediate behaviors. According to the above comparison, we can find that different boundary conditions do not influence the deformation mechanism of single crystal W and our conclusions also apply to nanowires.

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