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Supplementary Materials for

Dislocation behaviors in nanotwinned diamond

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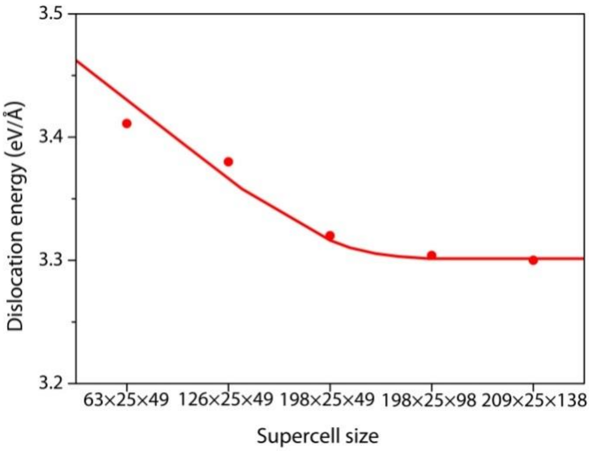


Fig. S1. Dislocation energy as function of supercell size.

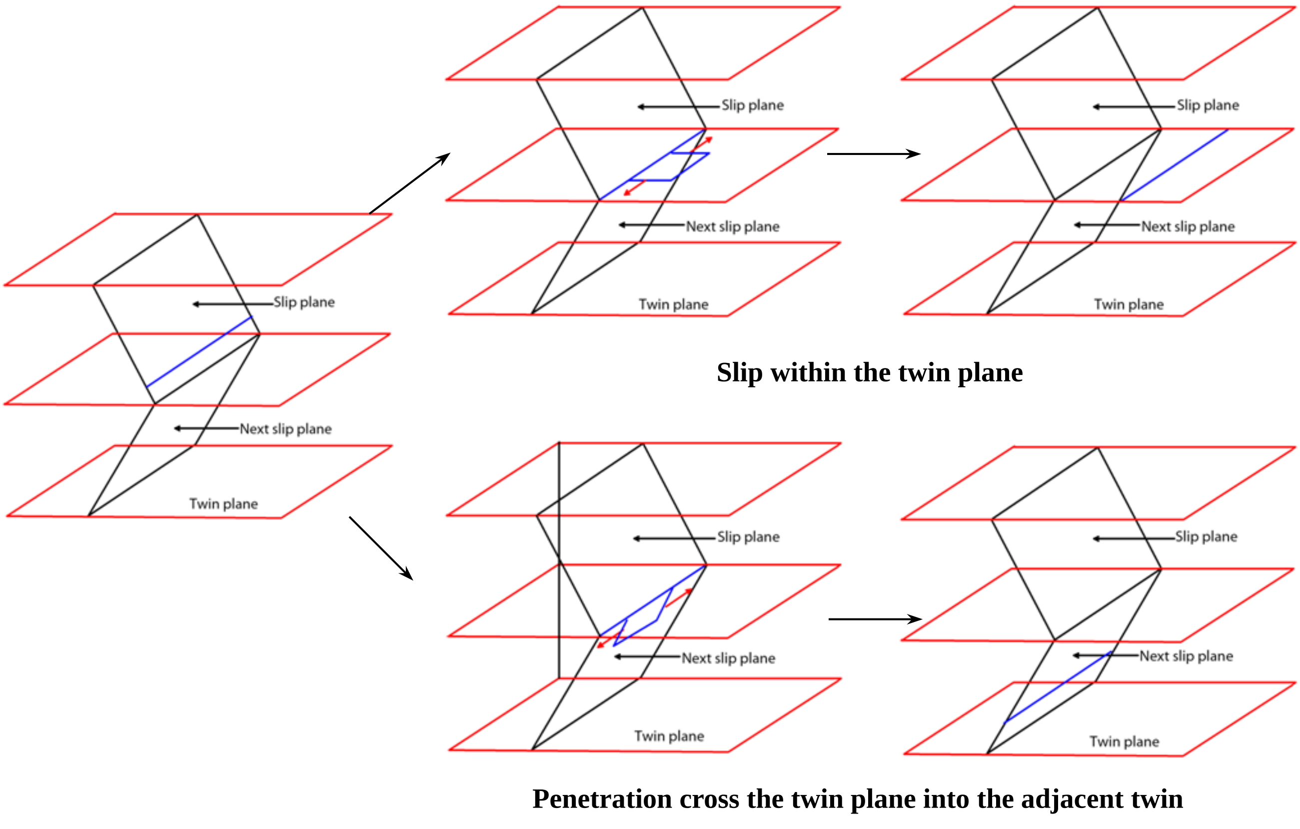
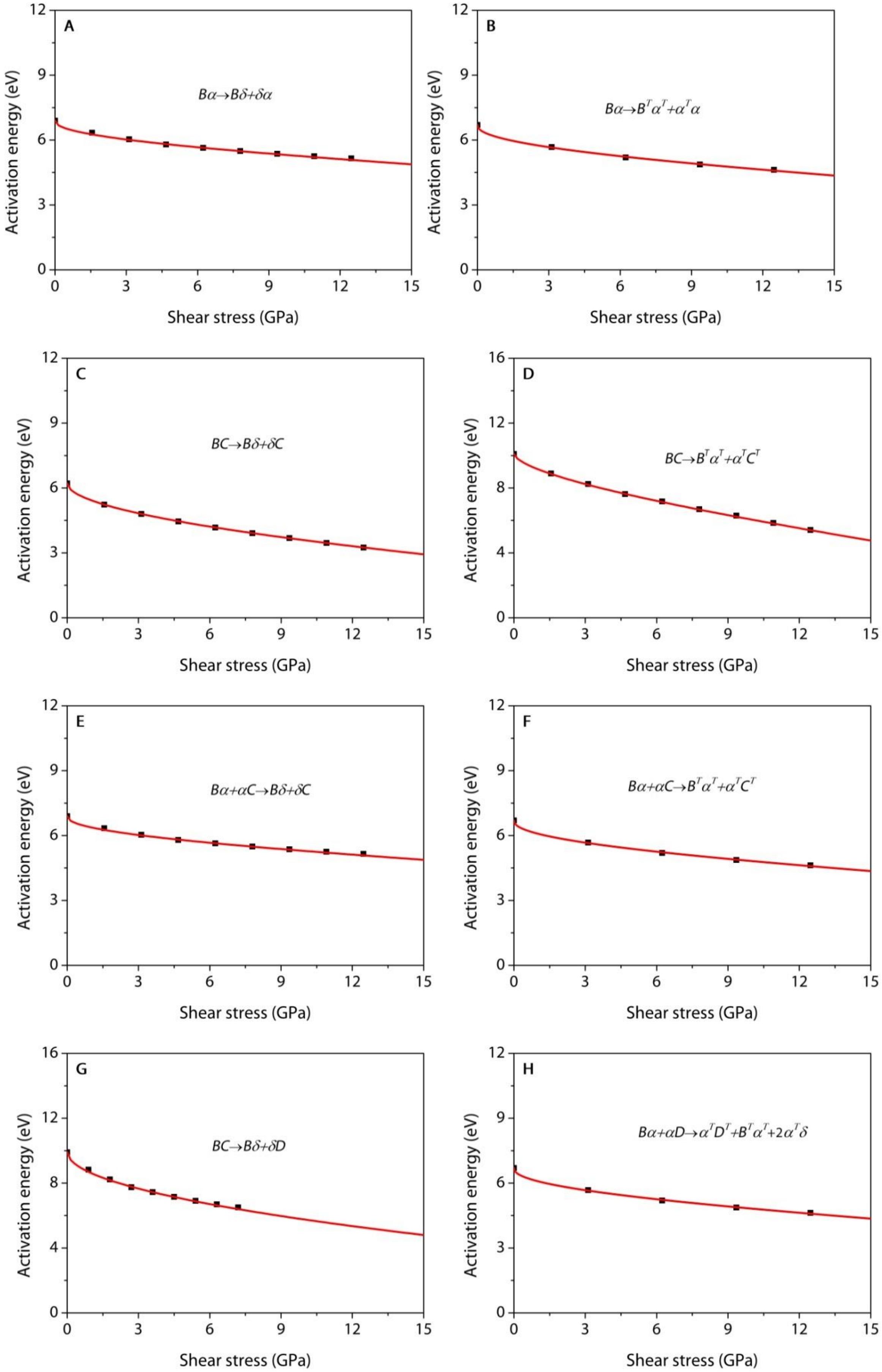


Fig. S2. Schematic of process for dislocation reaction with twin plane. The reaction involves formation of kinks, which migrate along the dislocation line.


A
$B\alpha \rightarrow B\delta + \delta\alpha$
B
$B\alpha \rightarrow B^T\alpha^T + \alpha^T\alpha$
C
$BC \rightarrow B\delta + \delta C$
D
$BC \rightarrow B^T\alpha^T + \alpha^T C^T$
E
$B\alpha + \alpha C \rightarrow B\delta + \delta C$
F
$B\alpha + \alpha C \rightarrow B^T\alpha^T + \alpha^T C^T$
G
$BC \rightarrow B\delta + \delta D$
H
$B\alpha + \alpha D \rightarrow \alpha^T D^T + B^T\alpha^T + 2\alpha^T\delta$
Activation energy (eV)
Shear stress (GPa)

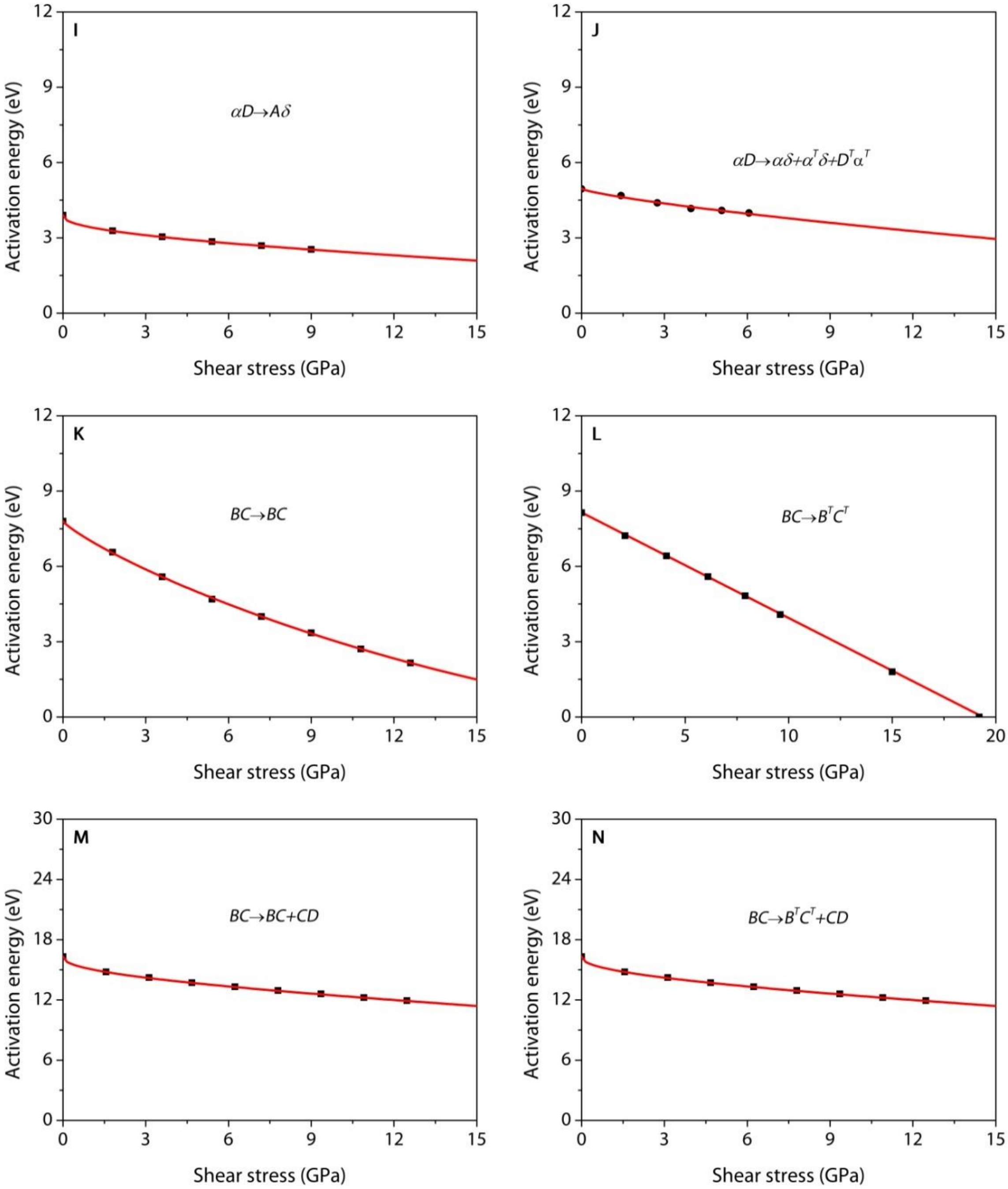


Fig. S3. Calculated shear stress–dependent activation energy of dislocation reaction with twin plane. (**A**)~(**B**) Shear stress dependent activation energy of glide-set 30° partial dislocation reaction with twin plane. (**C**)~(**F**) Shear stress dependent activation energy of glide-set 0° perfect dislocation reaction with twin plane. (**G**)~(**H**) Shear stress dependent activation energy of glide-set 60° perfect dislocation reaction with twin plane. (**I**)~(**J**) Shear stress dependent activation energy of glide-set 90° partial dislocation reaction with twin plane. (**K**)~(**L**) Shear stress dependent activation energy of shuffle-set 0° perfect dislocation reaction with twin plane. (**M**)~(**N**) Shear stress dependent activation energy of shuffle-set 60° perfect dislocation reaction with twin plane.

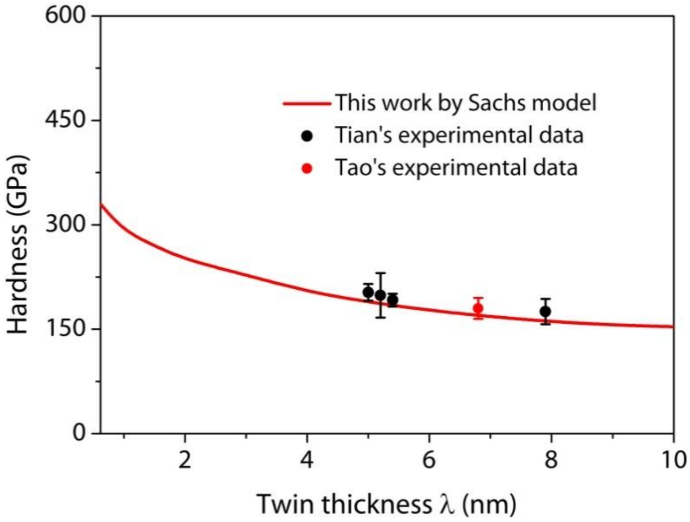


Fig. S4. Hardness of nt-diamond at grain size of 125 nm.

Table S1. Calculated kink energy E_f and activation energy W_m of kink migration for dislocation reactions by slip transfer mode.

Types of dislocation	Dislocation reactions equation	E_f(eV)	W_m (eV)	Activation energy (eV)
Glide-set 30° partial dislocation	$B\alpha \rightarrow B\delta + \delta\alpha$	2.2	2.5	6.9
	$B\alpha \rightarrow B^T\alpha^T + \alpha^T\alpha$	1.4	3.9	6.7
Glide-set 90° partial dislocation	$\alpha D \rightarrow A\delta$	0.5	2.9	3.9
	$\alpha D \rightarrow \alpha\delta + \alpha^T\delta + D^T\alpha^T$	0.5	3.6	4.6
Glide-set 0° perfect dislocation	$BC \rightarrow B\delta + \delta C$	2.8	0.6	6.2
	$BC \rightarrow B^T\alpha^T + \alpha^T C^T$	3.1	4.0	10.2
	$B\alpha + \alpha C \rightarrow B\delta + \delta C$	2.2	2.5	6.9
	$B\alpha + \alpha C \rightarrow B^T\alpha^T + \alpha^T C^T$	1.9	2.9	6.7
Glide-set 60° perfect dislocation	$BD \rightarrow B\delta + \delta D$	2.0	5.9	9.9
	$B\alpha + \alpha D \rightarrow \alpha^T D^T + B^T\alpha^T + 2\alpha^T\delta$	1.9	2.9	6.7
Shuffle-set 0° perfect dislocation	$BC \rightarrow BC$	3.4	1.0	7.8
	$BC \rightarrow B^T C^T$	3.5	1.2	8.2
Shuffle-set 60° perfect dislocation	$BD \rightarrow BC + CD$	5.1	6.1	16.3
	$BD \rightarrow B^T C^T + CD$	5.1	6.1	16.3

Table S2. Fitted parameters used in Eq. 10. Q_0 is the activation energy at temperature of 0 K and stress of 0 GPa, in eV; **p** and **q** are energy barrier shape parameters; τ_{TB} is barrier strength, in GPa.

Types of dislocation	Dislocation reactions equation	Q_0	p	q	τ_{TB}
Glide-set 30° partial	$B\alpha \rightarrow B\delta + \delta\alpha$	6.9	0.44	0.41	53.7
dislocation	$B\alpha \rightarrow B^T\alpha^T + \alpha^T\alpha$	6.7	0.44	0.49	52.1
Glide-set 90° partial	$\alpha D \rightarrow A\delta$	3.9	0.43	0.55	37.2
dislocation	$\alpha D \rightarrow \alpha\delta + \alpha^T\delta + D^T\alpha^T$	4.6	0.73	1.01	49.3
Glide-set 0° perfect	$BC \rightarrow B\delta + \delta C$	6.2	0.52	0.88	43.7
dislocation	$BC \rightarrow B^T\alpha^T + \alpha^T C^T$	10.2	0.62	0.75	31.7
	$B\alpha + \alpha C \rightarrow B\delta + \delta C$	6.9	0.44	0.41	53.7
	$B\alpha + \alpha C \rightarrow B^T\alpha^T + \alpha^T C^T$	6.7	0.44	0.49	52.1
Glide-set 60° perfect	$BD \rightarrow B\delta + \delta D$	9.9	0.52	0.99	55.3
dislocation	$B\alpha + \alpha D \rightarrow \alpha^T D^T + B^T\alpha^T + 2\alpha^T\delta$	6.7	0.44	0.49	52.1
Shuffle-set 0°perfect	$BC \rightarrow BC$	7.8	0.84	1.5	24.1
dislocation	$BC \rightarrow B^T C^T$	8.2	0.95	0.96	19.2
Shuffle-set 60°	$BD \rightarrow BC + CD$	16.3	0.43	0.39	47.7
perfect dislocation	$BD \rightarrow B^T C^T + CD$	16.3	0.43	0.39	47.7

Table S3. The parameters used to calculate the critical resolved shear stress of slip transfer mode, confined layer slip mode, and paralleled to twin plane slip mode. τ_0 is the lattice functional stress, in GPa; τ_{TB} is the barrier strength, in GPa; ν is Poisson's ratio; G is shear modules, in GPa; b is the magnitude of Burgers vector, in nm; p and q is are activation energy shape parameters for shuffle-set 0° perfect dislocation penetration twin plane; θ is angle between slip plane and twin plane, in degree; d is the grain size, in nm.

Parameters	τ_0	τ_{TB}	ν	G	b	p	q	θ	d
	10.3	19.2	0.078	540	0.25	0.95	0.96	70.5	20