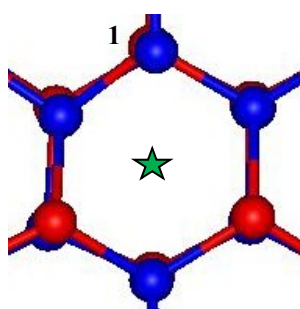


Supplementary Material

Detailed atomic structures of the core configurations of the **c**-type (S6, D6) and the **a**-type (S, G, G*) screw dislocations in indium nitride. Bond lengths (minimum, maximum and average) and bond angles (minimum, maximum and average) are listed for the five core configurations. The values in bold character refer to the bond lengths of In–In or N–N wrong bonds. Red balls represent indium atoms and blue balls represent nitrogen atoms. The green star represents the centre of the dislocation.

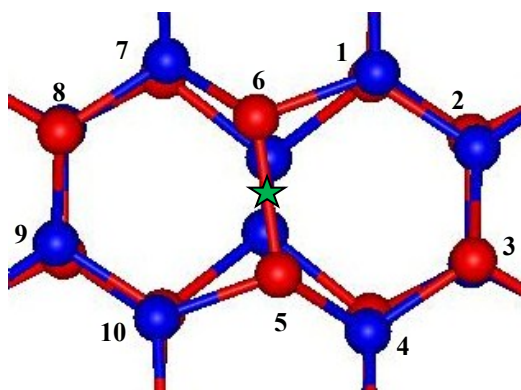
Configuration (S6):



* All the six atomic columns are equivalent.

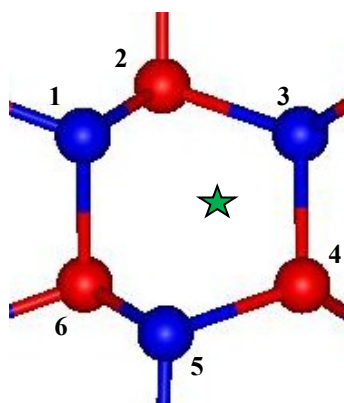
Column	Nature (Coordination number)	Bond length (Å)			Bond angles (°)		
		Min	Max	Av	Min	Max	Av
1	In (4)	2.13	2.49	2.26	78.5	133.3	109.9
	N (4)	2.14	2.53	2.27	79.3	133.8	109.1

Configuration (D6):



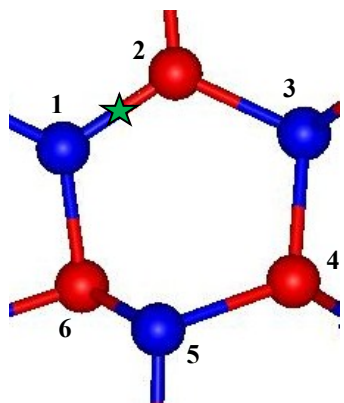
Column	Nature (Coordination number)	Bond length (Å)			Bond angles (°)		
		Min	Max	Av	Min	Max	Av
1	In (4)	2.16	2.31	2.23	82.7	126.9	109.1
	N (4)	2.15	2.21	2.18	89.8	123.1	109.4
2	In (4)	2.15	2.26	2.19	92.7	124.8	109.5
	N (4)	2.16	2.26	2.19	90.7	124.2	109.4
3	In (4)	2.17	2.26	2.21	87.4	127.0	109.4
	N (4)	2.15	2.26	2.20	88.2	127.8	109.2
4	In (4)	2.15	2.35	2.22	93.1	116.6	109.2
	N (4)	2.12	2.26	2.19	86.0	121.9	109.0
5	In (4)	2.19	2.69	2.42	74.1	135.6	107.5
	N (4)	1.27	2.88	2.51	66.2	128.5	105.4
6	In (4)	2.18	2.69	2.39	76.4	136.0	107.7
	N (4)	1.27	2.78	2.48	67.9	126.6	106.1
7	In (4)	2.15	2.35	2.22	93.0	116.4	109.2
	N (4)	2.12	2.25	2.19	86.8	122.0	108.9
8	In (4)	2.17	2.25	2.21	87.8	126.6	109.5
	N (4)	2.15	2.26	2.20	88.6	127.4	109.2
9	In (4)	2.15	2.26	2.19	93.1	124.4	109.4
	N (4)	2.16	2.27	2.20	91.0	123.8	109.4
10	In (4)	2.17	2.32	2.23	82.3	128.1	109.0
	N (4)	2.15	2.20	2.17	90.5	124.0	109.3

Configuration (S):



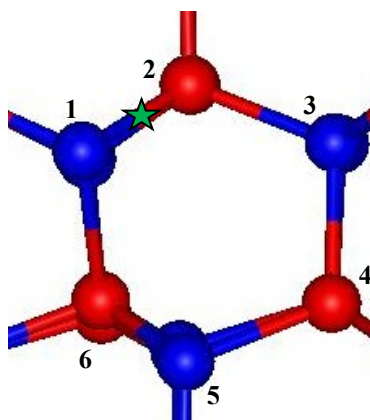
Column	Nature (Coordination number)	Bond length (Å)			Bond angles (°)		
		Min	Max	Av	Min	Max	Av
1	N (4)	2.16	2.26	2.21	90.9	125.1	108.8
2	In (4)	2.16	2.26	2.21	91.8	130.8	108.8
3	N (4)	2.22	2.27	2.24	90.9	130.7	110.1
4	In (4)	2.19	2.27	2.23	89.5	131.7	110.2
5	N (4)	2.16	2.28	2.22	91.5	132.4	108.5
6	In (4)	2.15	2.28	2.21	91.3	125.3	108.9

Configuration (G):



Column	Nature (Coordination number)	Bond length (Å)			Bond angles (°)		
		Min	Max	Av	Min	Max	Av
1	N (3)	1.99	2.08	2.05	114.9	125.4	119.9
2	In (3)	1.99	2.14	2.08	119.2	121.0	120.0
3	N (4)	2.12	2.23	2.18	97.6	123.0	109.6
4	In (4)	2.16	2.20	2.18	104.0	120.0	109.3
5	N (4)	2.16	2.21	2.18	100.0	124.5	109.2
6	In (4)	2.08	2.21	2.17	98.4	121.7	109.0

Configuration (G*):



Column	Nature (Coordination number)	Bond length (Å)			Bond angles (°)		
		Min	Max	Av	Min	Max	Av
1	N (4)	1.41	2.43	2.26	85.5	128.5	108.7
2	In (4)	2.17	3.01	2.18	88.0	129.1	109.3
3	N (4)	2.16	2.22	2.19	96.2	121.9	109.7
4	In (4)	2.18	2.22	2.19	96.4	120.8	109.7
5	N (4)	2.15	2.18	2.16	99.3	123.4	109.3
6	In (4)	2.15	2.43	2.25	86.8	139.1	108.3