The remarkable role of grain boundaries in the thermal transport properties of phosphorene

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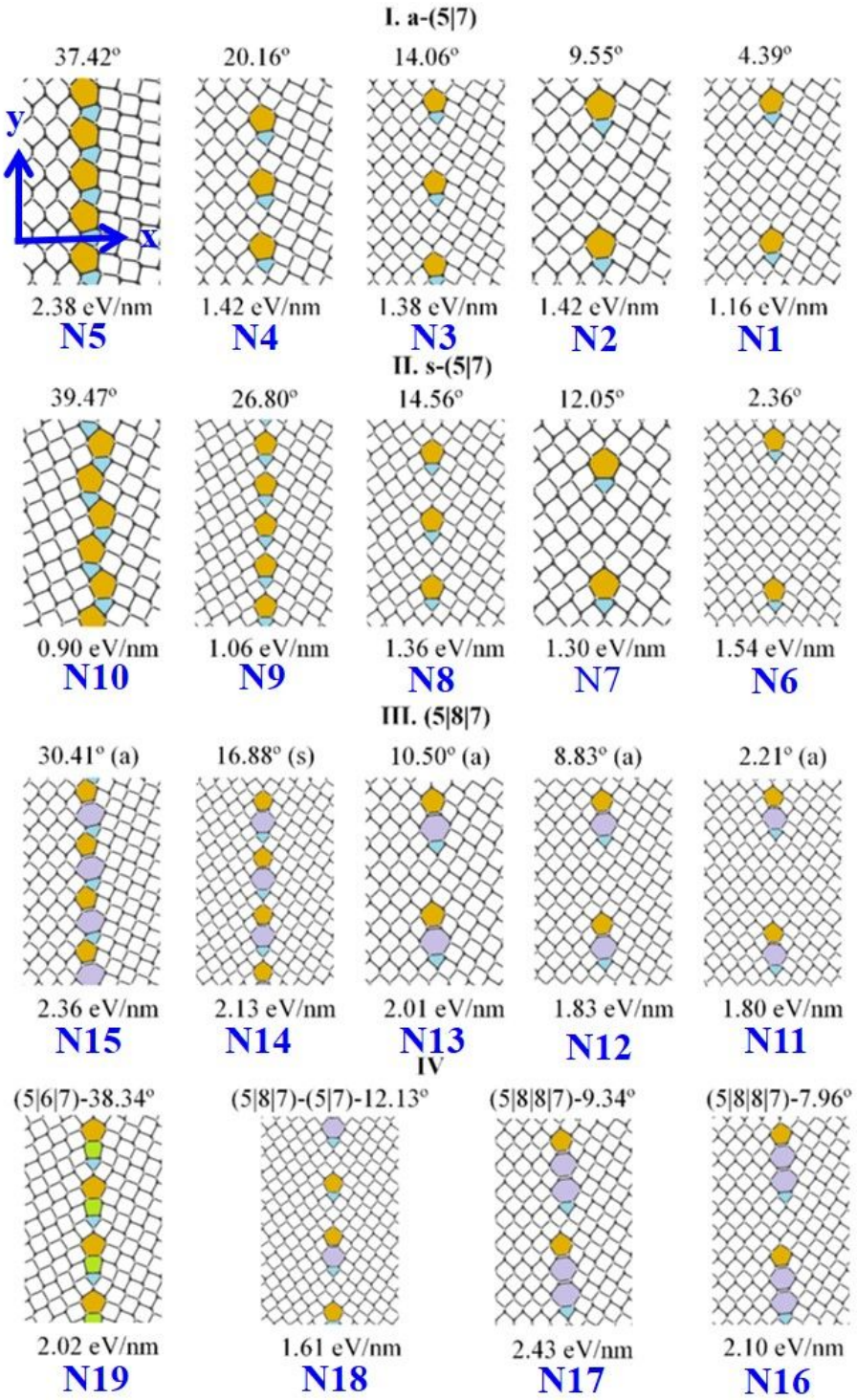

Figure S1. The structures of four types of phosphorene GBs. The misorientation angle and formation energy are also given. Smaller formation energy means easier to form the GB. Reprinted with permission from Ref. [24], copyright (2019) by the IOP Publishing.

Table S1. Structural parameters and thermal conductivities of four types of phosphorene GBs.

I. a-(5|7)	**N1**	**N2**	**N3**	**N4**	**N5**
θ	4.39º	9.55º	14.06º	20.16º	37.42º
d_H **(Å)**	23.45	18.63	14.11	9.59	5.43
κ_x **(Wm^{-1}K^{-1})**	37.5	35.0	29.5	20.3	14.5
κ_y **(Wm^{-1}K^{-1})**	7.0	6.6	6.3	7.3	10.3
II. s-(5|7)	**N6**	**N7**	**N8**	**N9**	**N10**
θ	2.36º	12.05º	14.56º	26.80º	39.47º
d_H **(Å)**	27.99	32.55	23.63	14.29	9.85
κ_x **(Wm^{-1}K^{-1})**	34.7	32.6	22.1	17.8	16.8
κ_y **(Wm^{-1}K^{-1})**	5.9	5.9	5.6	7.0	8.5
III. (5|8|7)	**N11**	**N12**	**N13**	**N14**	**N15**
θ	2.21º	8.83º	10.50º	16.88º	30.41º
d_H **(Å)**	27.99	23.26	18.91	23.60	9.51
κ_x **(Wm^{-1}K^{-1})**	16.1	14.0	12.0	9.3	7.9
κ_y **(Wm^{-1}K^{-1})**	4.6	4.4	4.5	4.3	4.1
IV. (5|6-8|7)	**N16**	**N17**	**N18**	**N19**	
θ	7.96º	9.34º	12.13º	38.34º	
d_H **(Å)**	23.34	18.75	28.09	9.86	
κ_x **(Wm^{-1}K^{-1})**	9.8	9.0	8.9	8.6	
κ_y **(Wm^{-1}K^{-1})**	2.9	2.9	2.5	2.6	

Table S2. Heat flux J, temperature jump ΔT, and thermal boundary resistances R in N5 GBs with different structure size.

Sample No.	$L_L=L_R$ (Å)	L_M (Å)	J ($\times 10^9$ Wm^{-2})	ΔT (K)	R ($\times 10^{-10}$ m^2KW^{-1})
1	361.4	464.6	3.49	3.46	9.93
2	722.8	464.6	2.68	2.55	9.52
3	722.8	836.3	2.49	2.52	10.13