

SUPPLEMENTARY MATERIAL

Hardness and Electronic Properties of Si-C-N Structures

Shuai Chen,^a Xiaogang Guo,^a Hefei Li,^a Pan Ying,^a Rongxin Sun,^a Mengdong Ma,^{a, b} Yingju Wu,^a

Lingjuan Hao,^c Dongli Yu,^a Julong He,^{a*} Yufei Gao,^{a*} and Yongjun Tian^a

^a Center for High Pressure Science (CHiPS), State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, 066004, China

^b Macao Institute of Materials Science and Engineering, Macau University of Science and Technology, Taipa, Macao 999078, China

^c Handan key Laboratory of Intelligent Awareness and Application, Handan University, Handan, 056001, China

* Author to whom correspondence should be addressed. E-mail address: hjl@ysu.edu.cn;
gyf@ysu.edu.cn

Table S1. Atomic Wyckoff positions of the SiC_3N_3 , SiC_7N_6 , and $\text{SiC}_{13}\text{N}_{14}$.

SiC_3N_3		SiC_7N_6		$\text{SiC}_{13}\text{N}_{14}$	
Atom	Wyckoff positions	Atom	Wyckoff positions	Atom	Wyckoff positions
Si_1	2a (0.00, 0.00, 0.47)	Si	2a (0.00, 1.00, 0.46)	Si	1a (0.00, 0.00, 0.90)
Si_2	2b (0.67, 0.33, 0.47)	C_1	6c (0.50, 0.58, 0.66)	C_1	1a (0.00, 0.00, 0.49)
C_1	6c (0.52, 0.59, 0.66)	C_2	6c (0.79, 0.09, 0.46)	C_2	3d (0.10, 0.80, 0.96)
C_2	6c (0.78, 0.08, 0.46)	C_3	6c (0.33, 0.67, 0.58)	C_3	3d (0.57, 0.49, 0.16)
N_1	6c (0.41, 0.09, 0.44)	N_1	3d (0.40, 0.07, 0.43)	C_4	3d (0.26, 0.18, 0.45)
N_2	6c (0.65, 0.02, 0.73)	N_2	3d (0.36, 0.35, 0.71)	C_5	3d (0.49, 0.57, 0.66)
				N_1	3d (0.66, 0.60, 0.43)
				N_2	3d (0.33, 0.33, 0.70)
				N_3	3d (0.59, 0.65, 0.94)
				N_4	3d (0.67, 0.00, 0.21)
				N_5	1b (0.33, 0.67, 0.57)
				N_6	1c (0.67, 0.33, 0.08)

Table S2. Chemical bond parameters and Vickers hardness of SiC₃N₃.

Bond type	<i>d</i> (Å)	Pop	<i>F_i</i>	<i>N_e</i>	<i>H^{x-y}_v</i> (GPa)	<i>H_v</i> (GPa)
C ₁ -Si ₂	1.93	0.64	0.40	0.32	5.12	28.04
C ₂ -Si ₁	1.95	0.66	0.41	0.31	14.35	
C ₁ -N ₁	1.43	0.80	0.31	0.89	57.35	
C ₁ -N ₁	1.55	0.62	0.49	0.71	32.72	
C ₁ -N ₂	1.51	0.65	0.43	0.77	38.07	
C ₂ -N ₁	1.49	0.66	0.46	0.79	36.15	
C ₂ -N ₂	1.48	0.77	0.28	0.80	44.16	
C ₂ -N ₂	1.47	0.73	0.28	0.82	45.70	

Table S3. Chemical bond parameters and Vickers hardness of SiC₇N₆.

Bond type	<i>d</i> (Å)	Pop	<i>F_i</i>	<i>N_e</i>	<i>H^{x-y}_v</i> (GPa)	<i>H_v</i> (GPa)
C ₂ -Si	1.86	0.67	0.35	0.32	15.43	31.17
C ₁ -C ₃	1.57	0.86	0.18	0.55	10.91	
C ₁ -N ₁	1.44	0.77	0.24	0.80	48.93	
C ₁ -N ₂	1.45	0.72	0.28	0.79	51.63	
C ₂ -N ₁	1.57	0.65	0.35	0.62	28.51	
C ₂ -N ₁	1.51	0.64	0.47	0.69	29.25	
C ₂ -N ₂	1.45	0.77	0.29	0.78	48.25	
C ₂ -N ₂	1.46	0.83	0.22	0.78	52.09	

Table S4. Chemical bond parameters and Vickers hardness of SiC₁₃N₁₄.

Bond type	d (Å)	Pop	F_i	N_e	H^{x-y}_v (GPa)	H_v (GPa)
C ₁ -N ₁	1.50	0.74	0.26	0.69	40.30	40.64
C ₁ -N ₂	1.44	0.75	0.26	0.79	59.54	
C ₁ -N ₃	1.44	0.79	0.21	0.78	51.51	
C ₁ -N ₅	1.52	0.72	0.16	0.67	22.85	
C ₂ -N ₁	1.50	0.74	0.25	0.70	41.83	
C ₂ -N ₂	1.48	0.79	0.21	0.72	55.16	
C ₂ -N ₄	1.46	0.81	0.19	0.75	49.93	
C ₂ -C ₅	1.59	0.78	0.07	0.51	47.09	
C ₃ -N ₁	1.45	0.78	0.23	0.77	49.81	
C ₃ -N ₃	1.50	0.77	0.21	0.69	37.26	
C ₃ -N ₄	1.45	0.76	0.26	0.77	48.12	
C ₃ -N ₆	1.52	0.71	0.16	0.67	30.17	
C ₄ -Si	1.78	0.68	0.26	0.36	18.74	
C ₄ -N ₂	1.45	0.82	0.24	0.77	54.56	
C ₄ -N ₃	1.49	0.63	0.47	0.70	27.16	
C ₄ -N ₄	1.42	0.78	0.29	0.82	48.24	

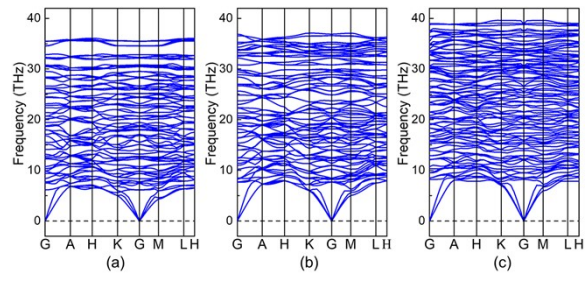


Figure S1. Phonon dispersion curves of (a) SiC_3N_3 , (b) SiC_7N_6 , and (c) $\text{SiC}_{13}\text{N}_{14}$