substance: boron compounds with group IV elements
property: boron carbonitrides, ternary system boron-carbon-silicon

B-C-N compounds.

Proposed scheme of the structure consisting of boron nitride and carbon layers in Fig. 1 [95H].

Preparation and properties of a compound in the B-C-N system [95H].

On the nature of boron-carbon-nitrogen compounds synthesized from organic precursors (comparison of NMR spectra of boron carbide, amorphous B and hexagonal boron nitride) [95A].

Preparation of BCN films in [94N].

High-temperature synthesis and investigation of hexagonal boron carbonitride [94A2, 93M1]; see also [94A1].

lattice parameters

Compound	*a* [Å]	*c* [Å]		
BCN		6.845		71K
	2.5	6.60		86D
BC_2N	~2.5	6.8		89K
	2.44	6.8		89L
		7.08		93M2
$(BN)_{0.26}C_{0.74}$	2.462(2)	6.79(1)		72R
BC_3N		7.2		93M1
$B_{1.1...1.3}C_{3.8...4.3}N$	2.440	6.658		91B
B_2C_5N	2.479	6.764		91S
"phase 1"		6.91		94A2
"phase 2"		6.715(1)...6.712(1)	partial N_2 pressure 50 to 30 %	
"phase 3"		6.704(1) Å	partial N_2 pressure 30 to 10 %	
"phase 4"		6.684(1) Å	partial N_2 pressure 5 %	

It is assumed that bond lengths found in hBCN should be consistent with those in graphite, hBN and graphite-like BC_3 (d_{BC} = 1.55 Å); the anticipated radii of the atomic species are as follows: r_B = 0.84 Å; r_C = 0.71 Å; r_N = 0.61 Å. In that event it is not unreasonable to expect the *a* value for BC_xN to be larger than in graphite and smaller than in hBN, since the ternary hybride can be treated as the substitutional solution either of carbon atoms in hBN or equal amounts of B and N atoms (with an averaged radius of 0.73) in graphite [94A2].

Lattice dynamics of a layered material BC_2N and calculated phonon density-of-states spectra [96N].

Electronic properties

Substitution patterns of the unit cells of layered BC_2N ($B_2C_4N_2$) types I, II and III in Fig. 2 [90L].

Brillouin zone of BC_2N ($B_2C_4N_2$) in Fig. 3 [90L].

Calculated electronic band structures of BC_2N ($B_2C_4N_2$), types I, II and III in Fig. 4 [89L].

Density of states calculation in Fig. 5 [89L].

Determination of the electronic structure, the band gap, the ionicity character, the lattice parameter and the bulk modulus by use of the empirical pseudopotential method associated with the virtual crystal approximation (VCA). VCA treats the $C_x(BN)_{1-x}$ as an alloy like a perfect crystal with an average potential at each sublattice site and does not include in lowest order the effects of aperiodic fluctuations in the crystal potentials [99Z].

Visible-light-emitting layered BC_2N semiconductor [96W].

For semiconductor properties see also [87K, 91S].

Structural and electronic properties of layered BC_2N in [95I].

Optical properties

Infrared spectra of different B – C – N compounds in Fig. 6 [95H].

Ternary system boron-carbon-silicon

For chemical, structural, and technological properties, see [72K].

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Fig. 1.

B-C-N compounds (BC_4N). Proposed scheme of boron nitride and carbon layers [95H].

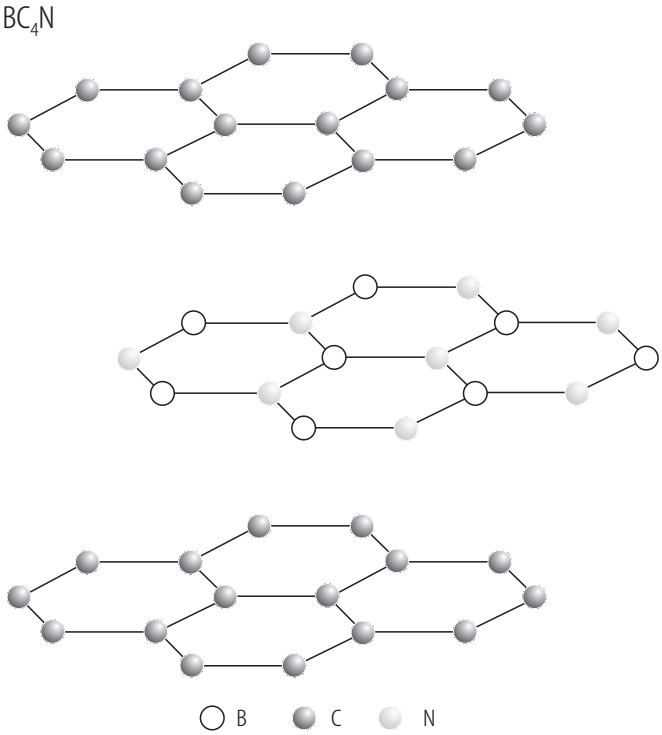
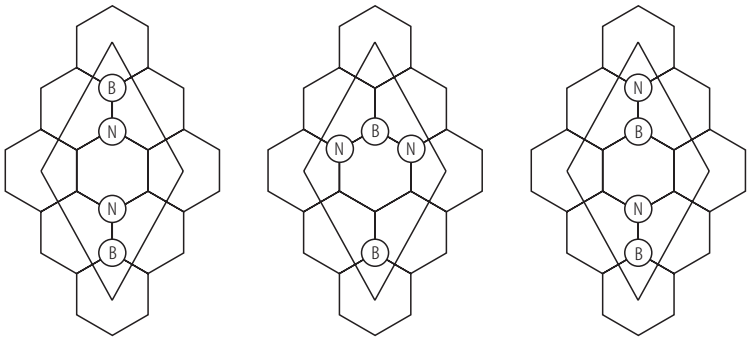


Fig. 2.

BC_2N ($B_2C_4N_2$). Substitution patterns of the unit cells of **(a)** type I, **(b)** type II and **(c)** type III [90L].



a $B_2C_4N_2(I)$ b $B_2C_4N_2(II)$ c $B_2C_4N_2(III)$

Fig. 3.

BC_2N ($B_2C_4N_2$). Brillouin zone for type III [90L].

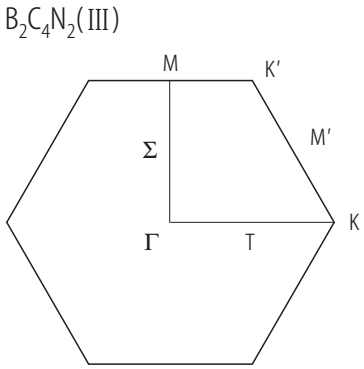


Fig. 4.

BC_2N ($B_2C_4N_2$). Calculated electronic band structures of **(a)** type I, **(b)** type II and **(c)** type III. The heavier lines indicate π bands, and the dashed horizontal lines mark the Fermi level [89L].

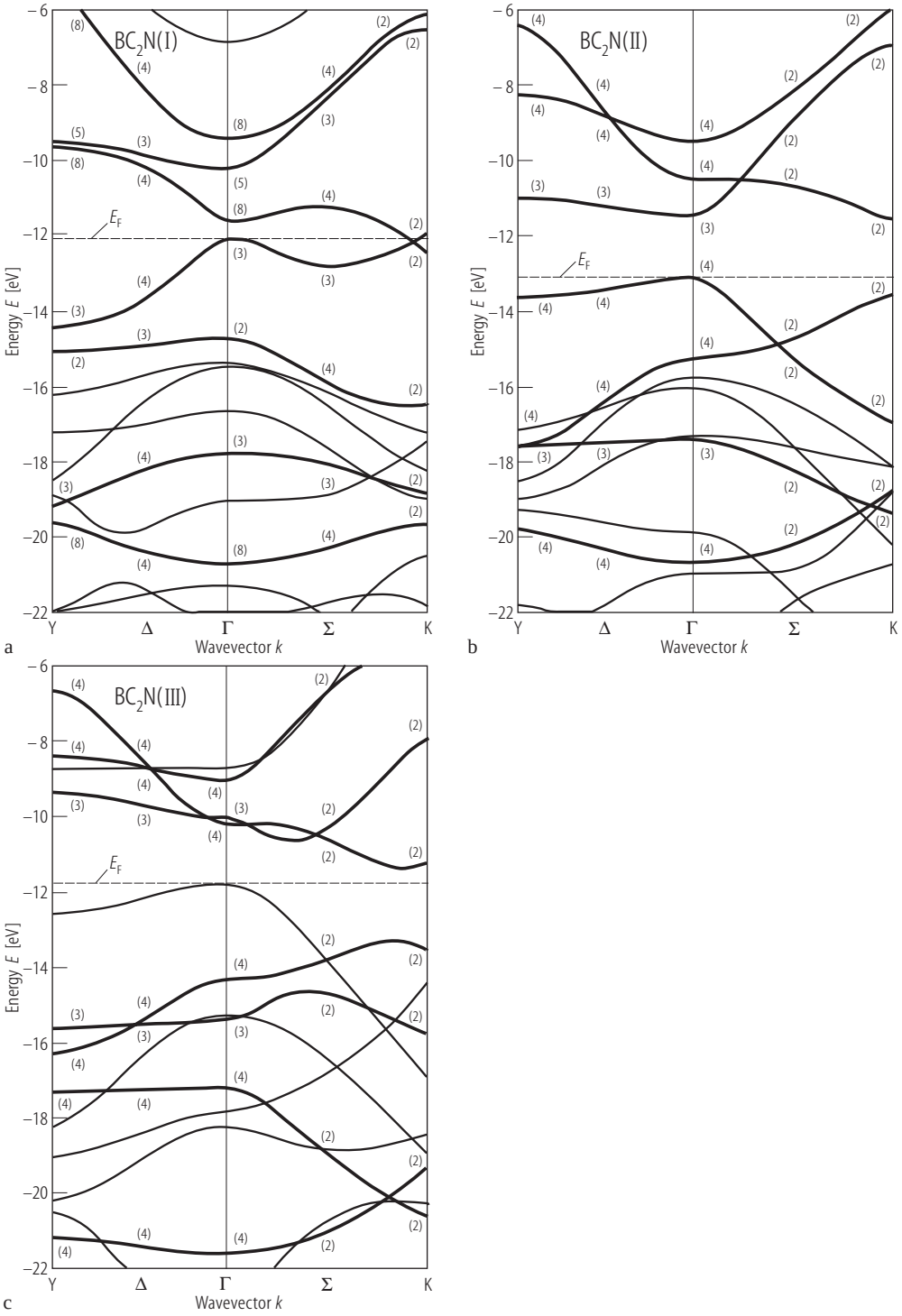


Fig. 5.

BC_2N ($B_2C_4N_2$). Calculated total and partial density of states for type II. The position of the Fermi level is indicated by the dashed line [89L]. Peaks 1 and 2 are composed of π states, while peak 3, which is about 6 eV higher in energy than peak 1, corresponds to the lowest-energy σ states above the Fermi level. Of the two π peaks the lower-energy one contains mainly N and C states; the higher-energy one contains mostly B and C states.

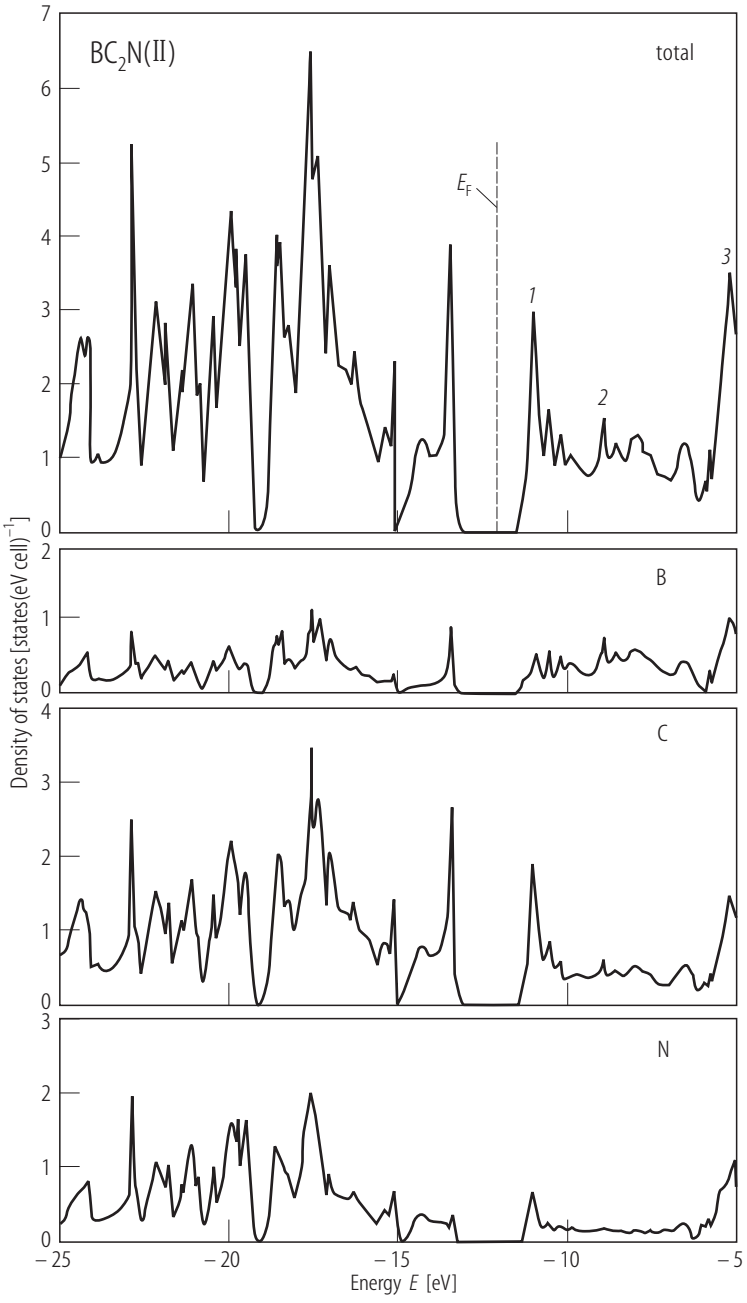


Fig. 6.

B-C-N compounds. IR transmission spectra of **(a)** samples prepared by mechanical mixtures of the two constituents obtained from the fused mixture of boric acid with urea (tBN) and saccharose with urea, respectively: (I) 10 % C, (II) 50 % C; (III) 70 % C, and **(b)** samples prepared from a fused mixture of boric acid and urea with varying saccharose ratios (I) 3.9 % C; (II) 32.6 % C; (III) 64.28 % C. Preparation temperature 1500 °C [95H].