Dispersion of Vibrational and Electronic States and Fine Spin-Dependent Structure of Their Energy Levels in Hexagonal BN Crystals and Nitrid-Borene

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Crystal structure of hexagonal graphite-like boron nitride h (γ) - BN and its single-layer nitroborene $BN_{L,1}$, their Brillouin zones and basic elements of symmetry

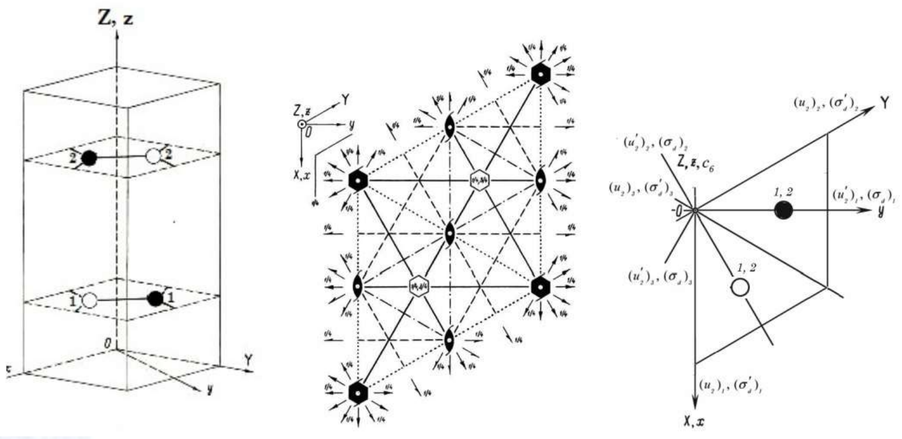


Figure 1. Structure of standard unit cell of hexagonal crystalline boron nitride h (γ) - BN *(a);* the standard diagramme of the spatial symmetry group $P6_3/mmc$ (D_{6h}^4) (b); orientation of the elements of the point symmetry group 6/mmm (D_{6h}) (c). The circles indicate the positions of the atoms of boron (dark) and nitrogen (transparent).

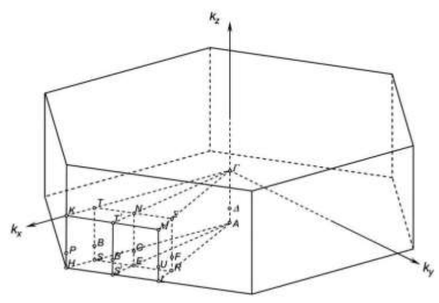


Figure 2. Brillouin zone of h (γ) - BN crystals and its symmetry points

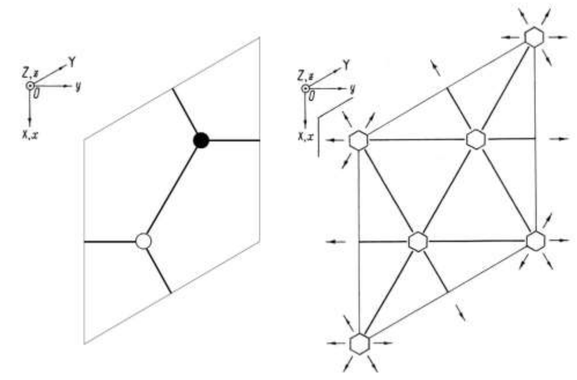
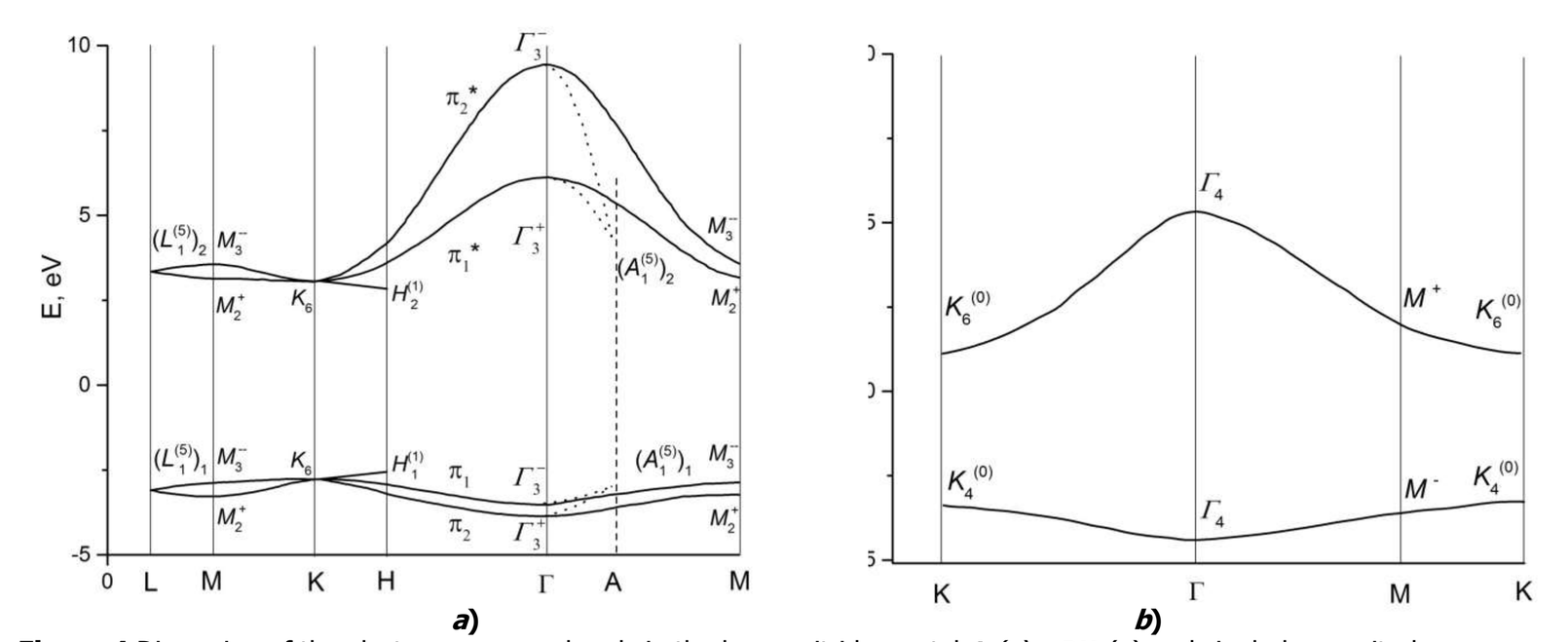


Figure 3. Structure of the sandard unit cell of single-layer nitro-borene $BN_{L,1}$ (*a*); the diagramm of the spatial symmetry group *DG78* (b). The circles indicate the positions of the atoms of borene (dark) and nitrogen (transparent).



a) ***b)***

Figure 4 Dispersion of the electron energy π-bands in the boron nitride crystal h (γ) - BN (a) and single-layer nitroborene $BN_{L,1}$ (letters mark the points in the Brillouin zone, and indexed letters do the irreducible projective representations of the corresponding projective classes)

Table 1 Irreducible projective representations of the K point of the nitrid-borene monolayer (BN) $_{L,1}$

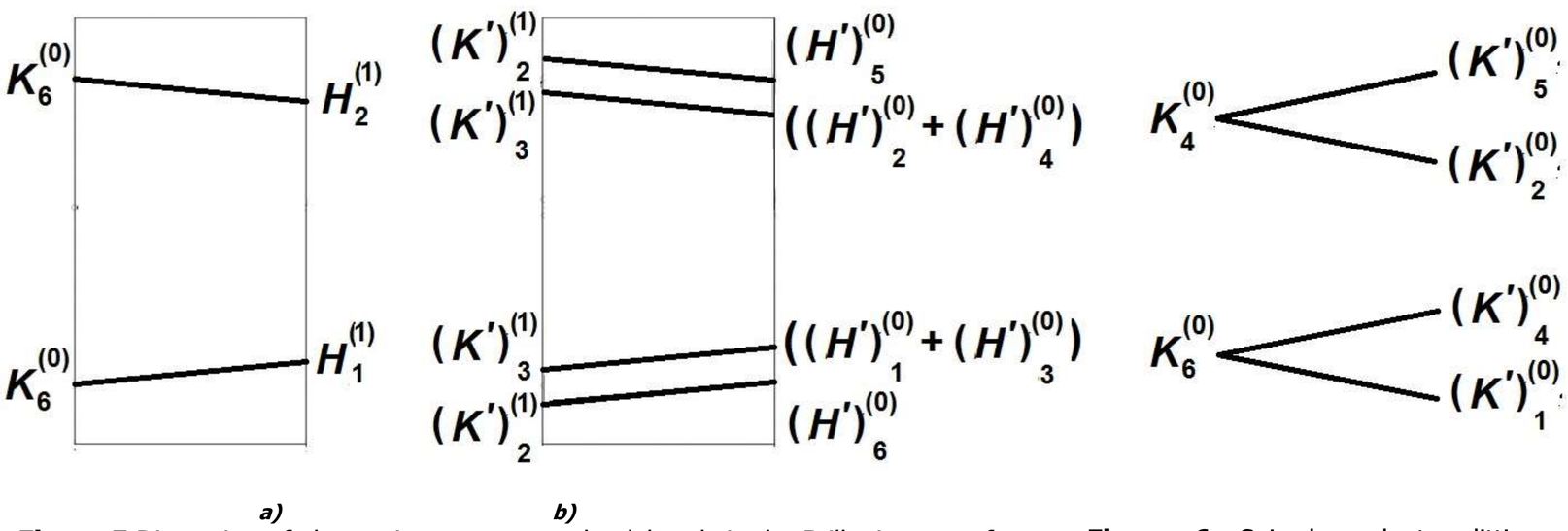
(C_{3h})	e	c_3	c_3^2	ic_2	ic_6^5	ic_6
$K_1^{(0)}$	1	1	1	1	1	1
$K_2^{(0)}$	1	1	1	−1	−1	−1
$K_3^{(0)}$	1	ϵ_3	ϵ_3^{-1}	1	ϵ_3	ϵ_3^{-1}
$K_4^{(0)}$	1	ϵ_3	ϵ_3^{-1}	−1	$-\epsilon_3$	$-\epsilon_3^{-1}$
$K_5^{(0)}$	1	ϵ_3^{-1}	ϵ_3	1	ϵ_3^{-1}	ϵ_3
$K_6^{(0)}$	1	ϵ_3^{-1}	ϵ_3	−1	$-\epsilon_3^{-1}$	$-\epsilon_3$

Table 2 Irreducible projective representations of the K point of the nitrid-borene monolayer (BN) $_{L,1}$ (taking into account electrone spin)

$\bar{6}\ (C_{3h})$	e	c_3	c_3^2	ic_2	ic_6^5	ic_6
$(K')_1^{(0)}$	1	−1	1	i	$-i$	$-i$
$(K')_2^{(0)}$	1	−1	1	$-i$	i	i
$(K')_3^{(0)}$	1	$-\epsilon_3$	ϵ_3^{-1}	i	ϵ_{12}	$-\epsilon_{12}^{-1}$
$(K')_4^{(0)}$	1	$-\epsilon_3$	ϵ_3^{-1}	$-i$	$-\epsilon_{12}$	ϵ_{12}^{-1}
$(K')_5^{(0)}$	1	$-\epsilon_3^{-1}$	ϵ_3	i	$-\epsilon_{12}^{-1}$	ϵ_{12}
$(K')_6^{(0)}$	1	$-\epsilon_3^{-1}$	ϵ_3	$-i$	ϵ_{12}^{-1}	$-\epsilon_{12}$

Table 3 Representation of electronic π-zones of the γ-BN monolayer ($(BN)_{L,1}$)

$\bar{6}\ (C_{3h})$	e	c_3	c_3^2	ic_2	ic_6^5	ic_6
K_{eq}	2	−1	−1	2	−1	−1
K_z	1	1	1	−1	−1	−1
K_π	2	−1	−1	−2	1	1
$K_{\mathbf{r}}$	3	0	0	1	−2	−2
K_{vib}	6	0	0	2	2	2
$D_{1/2}^+$	2	1	−1	0	$-\sqrt{3}$	$\sqrt{3}$
K_π'	4	−1	1	0	$-\sqrt{3}$	$\sqrt{3}$



a) ***b)***

Figure 5 Dispersion of electronic energy π- and π *-bands in the Brillouin zone of hexagonal crystalline graphite γ-C along the line $K-P-H$: without taking (a) and taking the electron spin into account (b)

Figure 6. Spin-dependent splitting of energy levels of electronic π -bands in single-layer nitroborene $BN_{L,1}$: π-states without taking (left) and taking the electron spin into account (right)

CONCLUSIONS

For the first time, projective classes are identified and the characters of irreducible projective representations are calculated, which characterize the symmetries of vibrational and electronic excitations without taking into account and taking it into account the electron spin for different points of the Brillouin zones of hexagonal boron nitride γ-BN and one-layer nitrid-borene $(BN)_{L,1}$.

Distributions on irreducible projective representations of vibrational excitations and electronic states determined by the structure of electronic π-zones for points of high symmetry of the corresponding Brillouin zones are found.

The dispersion of electronic excitations and the structure and symmetry of their spin-dependent fissures, which occur taking into account the electron spin, are qualitatively established.