Synthesis of Ternary B$_x$C$_y$N$_z$ Compounds from Thermolysis of 1,2 – Diamineborane towards hybrid BCN monolayer

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Graphene vs h-BN

Graphene

No Gap
Metallic

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Graphene vs h-BN

Graphene

Isostructural
2\% lattice constant mismatch

h-BN

Isoelectronic

No Gap
Metallic

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Graphene vs h-BN

Graphene

- No Gap
- Metallic

h-BN

- Bandgap
- Insulator

Isoelectronic

Isostructural
2% lattice constant mismatch

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Hybrid BCN systems

Growing of hybrid Gr and h-BN layer

Hybridized $h\text{-}B\text{N}_{x\times x\times y}$ structures would have interesting properties combining graphene and h-BN properties.
Hybrid BCN systems

Growing of hybrid Gr and h-BN layer
Hybridized h-BN$_{x}N_{x}C_{y}$ structures would have interesting properties combining graphene and h-BN properties

Electronic properties
Hybrid BCN systems

Growing of hybrid Gr and h-BN layer
Hybridized $h$-$B_N\;C_y$ structures would have interesting properties combining graphene and h-BN properties

Electronic properties

Structural configuration
Hybrid BCN systems

Growing of hybrid Gr and h-BN layer

Hybridized $h-B_{x}N_{x}C_{y}$ structures would have interesting properties combining graphene and h-BN properties.

Electronic properties


Problems: Phase segregation

“Pure” bonds are preferred to hybrid ones

Growth of atomic layer

Epitaxial growth by precursor decomposition on transition metal surfaces

500 - 1000°C
Growth of atomic layer

Epitaxial growth by precursor decomposition on transition metal surfaces

- Methane
- Ethane
- Ethylene

Graphene

500 - 1000°C
Growth of atomic layer

Epitaxial growth by precursor decomposition on transition metal surfaces

500 - 1000°C

Ammonia Borane
Borazine
Similar to benzene Liquid and not stable at room temperature
Stable at ambient conditions

Graphene
Methane
Ethane
Ethilene

h-BN

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Growth of atomic layer

Epitaxial growth by precursor decomposition on transition metal surfaces

500 - 1000°C

Metal

H desorption

Atomic layer

Pressure $2 \cdot 10^{-1} \text{ mbar}$
Methane    Ammonia Borane

Copper

1000°C

Ci et al. Nature Mat.. 2010, 9, 430

Methane

Ethane

Ethilene

Borazine
Similar to benzene Liquid and not stable at room temperature

Ammonia Borane
Stable at ambient conditions

Graphene

h-BN
EDAB solid phase characterization

Use a single precursor containing B, C and N atoms instead of two different precursors (one for graphene and one for h-BN)

Ethylenediamine Bisborane (EDAB)

\[ \text{BH}_3\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2\text{BH}_3 \]

Crystalline at room temperature

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EDAB at high temperature

In vacuum thermolysis $10^{-4}$ mbar

![EDAB](image)
EDAB at high temperature

In vacuum thermolysis $10^{-4}$ mbar

$H_2$ desorption events at 108°C, 157°C, and polymerization


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EDAB at high temperature

In vacuum thermolysis $10^{-4}$ mbar

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Desorption peaks at 231°C and 550°C
EDAB at high temperature

In vacuum thermolysis $10^{-4}$ mbar

$200^\circ C$  
EDAB  
Polymerization  
$1000^\circ C$  
Graphitization

$H_2$ desorption events at 108°C, 157°C, and polymerization

Desorption peaks at 231°C and 550°C
Presence of flake-like regions with sharp edges or compact areas
EDAB at high temperature

XRD broad peaks $2\theta = 24.2^\circ, 43.0^\circ$ of a poorly crystalline graphitic phase
EDAB at high temperature

XRD broad peaks $2\theta = 24.2^\circ$, $43.0^\circ$ of a poorly crystalline graphitic phase

Sharp diffraction peaks assigned to Ammonium Hydroxide Borate Hydrate (or Ammonium Borate Hydrate $\text{B}_5\text{H}_{12}\text{NO}_{12}$), graphite and $(\text{BN})_{0.26} \text{C}_{0.74}$
EDAB at high temperature

Energy X-ray dispersive analysis (EDX) shows mixing of B, C, N

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EDAB at high temperature

C 1s from sp3 to sp2 hybridization (284.4 eV)

Wilson et al. Nano Research 2013, 6, 99
EDAB at high temperature

C 1s from sp3 to sp2 hybridization (284.4 eV)

Presence of hybrid C – N and C – B bonds

Ci et al. Nature Mat.. 2010, 9, 430

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N 1s (399.2 eV) in agreement with presence of B-N and C-N coordination
EDAB at high temperature

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Wilson et al. Nano Research 2013, 6, 99

N 1s (399.2 eV) in agreement with presence of B-N and C-N coordination
Ci et al. Nature Mat. 2010, 9, 430

B 1s (192.6 eV) in agreement with the presence of prevalent boron oxide mixed with B-N, B-C coordination

B : C : N = 0.2 : 1 : 0.4
Conclusions

Formation of hybrid BCN is a new challenge for scientist providing a new class of monolayer material with tunable electronic structure
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Formation of hybrid BCN is a new challenge for scientist providing a new class of monolayer material with tunable electronic structure

We demonstrate formation of poor crystalline graphitic phase with B and N doping, from high temperature thermolysis of a single molecular precursor (EDAB)
Thank you for your attention