Ab initio Study of Partial Basal Dislocations in Bilayer Graphene

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Nuclear Graphite

• Synthetic polycrystalline graphite

• Neutron moderator and reflector

• Extremely high purity up to 99.97%

• Ability to withstand high temperatures

• Low neutron absorption cross-section

• High neutron scattering cross-section
UK Electricity Production

Department for Business, Energy & Industrial Strategy 27.08.2019
Irradiated Nuclear Graphite

• Crystal defects\textsuperscript{1,2}
  • 0d - Point defects
  • 1d - Line defects
    • Dislocations
  • 2d - Grain boundaries

• Irradiation effects\textsuperscript{1,2}
  • Dimensional Change
  • Irradiation Creep
  • Wigner Effect

1. R H Telling & M I Heggie, 2007
Dimensional Change

- Basal expansion up to 30% and in-plane shrinking up to 5\%\(^2\)

- **Prof. Malcolm Heggie**: New model for the dimensional change of the nuclear graphite\(^1\)
  *Buckle, Ruck and Tuck*

- Buckling and folding of the graphene sheets due to a progressive pile up of partial basal dislocations\(^1\)

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Irradiated Nuclear Graphite

HRTEM micrographs of HOPG at 800 C. Specimen irradiated to 1.75 dpa.

- (a) Shows formation of complex carbon onion like structure
- (b) Shows the curling and closure of basal planes
- (c) Shows the rucking and tucking of basal planes
- (d) Shows basal plane separation, delamination and voids

1. Steve Johns et al. Carbon, 2019
Dislocation Theory

“One small step for the dislocation, but a giant leap for plasticity”
Dislocation Theory

- The plane across which shear occurs: **Slip plane**
- The line that separates slipped and unslipped regions: **Dislocation line**
- The direction and magnitude of slip: **Burgers vector** \( \mathbf{b} \)
- If \( \mathbf{b} \) normal to \( \mathbf{l} \) dislocation is **Edge**
- If \( \mathbf{b} \) parallel to \( \mathbf{l} \) dislocation is **Screw**
- Any other angle dislocation is **Mixed**
Why Bilayer Graphene?

1. In Bernal graphite dislocation movement is mainly restricted to the basal plane (0001)

2. Basal dislocations cannot escape enabling their confinement in crystals as thin as only two monolayers

3. The material of choice is bilayer graphene: the thinnest possible crystal in which such linear defects can be confined
Crystallographic Directions

- Zigzag $<11\bar{2}0>$
  - [1210]
  - [1120]
  - [2110]
  - [1210]

- Armchair $<\bar{1}100>$
  - [0110]
  - [1100]
  - [1100]
  - [0110]
Crystallographic Directions

\[
[1\bar{2}10] = [1\bar{1}00] + [0\bar{1}10]
\]

\[
[2\bar{1}10] = [1\bar{1}00] + [10\bar{1}0]
\]

\[
[1\bar{1}20] = [10\bar{1}0] + [01\bar{1}0]
\]

\[
[\bar{1}2\bar{1}0] = [01\bar{1}0] + [\bar{1}100]
\]

\[
[\bar{2}110] = [\bar{1}100] + [\bar{1}010]
\]

\[
[\bar{1}\bar{1}20] = [\bar{1}010] + [0\bar{1}10]
\]
Dislocation line along $[10\bar{1}0]$

1. Pure Edge

$$\frac{a}{3} [1\bar{2}10] = \frac{a}{3} [1\bar{1}00] + \frac{a}{3} [0\bar{1}10]$$

2. Pure Mixed $30^0$

$$\frac{a}{3} [2\bar{1}\bar{1}0] = \frac{a}{3} [1\bar{1}\bar{1}0] + \frac{a}{3} [1\bar{1}00]$$
Pure Edge Dissociation

\[
\frac{a}{3} [\overline{1}2\overline{1}0] = \frac{a}{3} [1\overline{1}00] + \frac{a}{3} [0\overline{1}10]
\]

Diagram showing partial 60° and partial -60°.
Pure Mixed $30^0$ Dissociation

\[ \frac{a}{3} [2\overline{1}10] = \frac{a}{3} [10\overline{1}0] + \frac{a}{3} [1\overline{1}00] \]
Dislocation line along [1\bar{2}10]

3. Pure Screw

\[
\frac{a}{3}[1\bar{2}10] = \frac{a}{3}[1\bar{1}00] + \frac{a}{3}[0\bar{1}10]
\]

4. Pure Mixed 60°

\[
\frac{a}{3}[2\bar{1}10] = \frac{a}{3}[10\bar{1}0] + \frac{a}{3}[1\bar{1}00]
\]
Pure Screw Dissociation

\[ \frac{a}{3} [\overline{1}210] = \frac{a}{3} [\overline{1}100] + \frac{a}{3} [0\overline{1}10] \]
Pure Mixed $60^0$ Dissociation

$$\frac{a}{3} [2\overline{1}10] = \frac{a}{3} [1\overline{0}10] + \frac{a}{3} [1\overline{1}00]$$

[Diagram showing lattice with AB, AC, partial edge, and partial $30^0$ notations]
Modelling Software

LAMMPS Molecular Dynamics Simulator

AIMPRO.abinitio

#InspiringWinners since 1909
Pure Edge Dissociation

\[ \frac{a}{3} [\overline{1}210] = \frac{a}{3} [1\overline{1}00] + \frac{a}{3} [0\overline{1}10] \]
Pure Edge dislocations

(a) Diagram showing Pure Edge dislocations and Partial 60° dislocations.

(b) Diagram with a hexagonal lattice and labels for dislocation lines.

(c) Graph showing Basal [Å] vs. Zigzag [nm], with a red sine wave and a blue curve.

(d) Graph showing d002 [Å] vs. Zigzag [nm], with a blue curve.
Screw Component analysis

(a) Disregistry [nm]
(b) Burgers vector distribution

Disregistry [nm]

Burgers vector distribution

Zigzag [nm]

9.2 nm

Loughborough University

#InspiringWinners since 1909
Edge Component analysis

(a) Disregistry [Å] vs. Zigzag [nm]
(b) Burgers vector distribution vs. Zigzag [nm]

9.8 nm
Pure Screw Dissociation

\[ \frac{a}{3} [1\bar{2}10] = \frac{a}{3} [1\bar{1}00] + \frac{a}{3} [0\bar{1}10] \]
Pure Screw Dissociation
## Conclusion

<table>
<thead>
<tr>
<th>Partial Type</th>
<th>Edge component</th>
<th>Screw component</th>
<th>Energy/line</th>
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<tbody>
<tr>
<td>Partial Edge</td>
<td>8.9 nm</td>
<td>0</td>
<td>1.45 eV/nm</td>
</tr>
<tr>
<td>Partial 60°</td>
<td>9.8 nm</td>
<td>9.2 nm</td>
<td>2.51 eV/nm</td>
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<td>Partial 30°</td>
<td>?</td>
<td>?</td>
<td>?</td>
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<tr>
<td>Partial Screw</td>
<td>0</td>
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![Diagram of dislocation lines and crystal structures](image-url)
The scientist does not study nature because it is useful.

He studies it because he delights in it, and he delights in it because it is beautiful.

If nature were not beautiful, it would not be worth knowing, and if nature were not worth knowing, life would not be worth living.

Jules Henri Poincare
AB and AC stacking domains in Bilayer Graphene

STEM - ADF image of a stacking boundary showing a full transition from AB to AC stacking

Lin et al. Nano Letters, 2013
The blue and red lines mark the dislocation cores with the corresponding Burgers vectors of type

\[ \vec{b} = \frac{1}{3} < \bar{1}100 > \]

AB and AC stacking domains in Bilayer Graphene

The energy landscape for interlayer translation in bilayer graphene

- (A) Van der Waals energy landscape
- (B) Horizontal line cut through the energy landscape along an armchair direction
- (C) and (D) Dark-field TEM images of bilayer graphene

Alden et al. PNAS, 2013
Exchange-Correlation Functional

Diffusion Quantum Monte Carlo: Lattice parameters and interlayer binding energy are best described by LDA$^{1,3}$

## LDA vs GGA for Graphite

### Lattice Parameters

<table>
<thead>
<tr>
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<th>a (Å)</th>
<th>c (Å)</th>
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<tr>
<td>LDA-PW92</td>
<td>2.446</td>
<td>6.632</td>
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<td>GGA-PBE96</td>
<td>2.465</td>
<td>7.526</td>
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<tr>
<td>Zhao <em>et al.</em> 1989</td>
<td>2.452</td>
<td>6.671</td>
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### Error %

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<th>a</th>
<th>c</th>
<th>C_{11}</th>
<th>C_{33}</th>
<th>vdw</th>
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<td>LDA-PW92</td>
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<td>0.6</td>
<td>5.4</td>
<td>1.6</td>
<td>33</td>
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<td>GGA-PBE96</td>
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<td>12.8</td>
<td>10.7</td>
<td>76.4</td>
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<td>Ref.</td>
<td>2.452</td>
<td>6.671</td>
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<td>36.5</td>
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### Elast. Const (GPa)

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<tr>
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<th>C_{11}</th>
<th>C_{12}</th>
<th>C_{33}</th>
<th>C_{44}</th>
<th>C_{13}</th>
<th>C_{11} + C_{12}</th>
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<td>201</td>
<td>35.9</td>
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<tr>
<td>GGA-PBE96</td>
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<td>1108</td>
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<td>Cousins <em>et al.</em> 2003</td>
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<tr>
<td>Mounet <em>et al.</em> 2005</td>
<td>1118</td>
<td>235</td>
<td>29</td>
<td>4.5</td>
<td>-2.8</td>
<td>1353</td>
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### Inter. Binding (meV/atom)

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<td>LDA-PW92</td>
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<td>GGA-PBE96</td>
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<tr>
<td>DFT-D^1/vdW-DF^2</td>
<td>-26 to -69</td>
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<td>Quantum M. Carlo^1</td>
<td>-18</td>
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Bilayer Graphene $\gamma$-surface

- **AB**: 0 meV/A$^2$
- **SP**: 0.8 meV/A$^2$
- **AC**: 0 meV/A$^2$
- **AA**: 8.3 meV/A$^2$
- **PP**: 3.6 meV/A$^2$
Partial Edge Dislocations

\[ \mathbf{b}_1 = \frac{1}{3}[\bar{1}010] \]

\[ \mathbf{b}_2 = \frac{1}{3}[10\bar{1}0] \]
Partial Edge Dislocations

![Graph a](image)

![Graph b](image)

![Graph c](image)

![Graph d](image)
Dislocation Core Width analysis

(a) Disregistry [nm] vs Armchair [nm]

(b) Burgers vector distribution vs Armchair [nm]

- Disregistry [nm]: 8.9 nm
- Burgers vector distribution: 8.9 nm
Burgers vector Distribution

<table>
<thead>
<tr>
<th>Supercell Size [atoms]</th>
<th>Length [nm]</th>
<th>FWHM [nm]</th>
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<tr>
<td>800</td>
<td>42</td>
<td>8.4551</td>
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<tr>
<td>1600</td>
<td>84</td>
<td>8.4952</td>
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<tr>
<td>2400</td>
<td>126</td>
<td>8.6134</td>
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<td>3200</td>
<td>169</td>
<td>8.8046</td>
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<table>
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<th>Method</th>
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<tr>
<td>MD, Lin et al. 2013</td>
<td>~10</td>
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<tr>
<td>Exp, Alden et al. 2013</td>
<td>6-11</td>
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