MOCVD Routes to 2D Crystals

Joan M. Redwing

Department of Materials Science & Engineering
Materials Research Institute
Center for Two-Dimensional and Layered Materials (2DLM)

The Pennsylvania State University
University Park, PA 16802 USA
Graphene-like layered materials

Exhibit wide variety of electronic properties – insulators, semiconductors, semi-metals, superconductors
The TMD Synthesis “Atlas”
Highly scalable process
Excellent control over W:Se ratio

Tungsten Diselenide ($\text{WSe}_2$)

- Defects serve as nucleation sites in 2D materials.
- Typical defects are chalcogen (S, Se, Te) vacancies.

Se:W ratio has significant impact on domain size, shape, and “defect” formation.

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>Time (min)</th>
<th>Pre-Anneal</th>
<th>Pressure (Torr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>800</td>
<td>30</td>
<td>500°C, 15min</td>
<td>700</td>
</tr>
</tbody>
</table>

Se:W Ratio: 170

Se:W Ratio: 400

Se:W Ratio: 800

Se:W Ratio: 14000

Se:W ratio has a significant impact on domain size, shape, and “defect” formation.
WSe$_2$ on Free Standing Graphene Templates

- Developed process to produce freestanding van der Waals heterostructures
- Ideal for investigating layer-layer interaction with graphene

WSe$_2$ – Epitaxy and Defects

(a) TEM image and (b) SAD pattern showing epitaxial relationship between WSe$_2$ and graphene
(c) Structural model showing alignment of W atoms in WSe$_2$ and C atoms in graphene (circled in red)

(a) HAADF-STEM image of monolayer and multilayer WSe$_2$
(b) HAADF-STEM images of (b) monolayer WSe$_2$ and (c) edge region showing W-termination
(d) TEM image showing nucleation near grain boundary in graphene
Pulsed MOCVD growth of GaN

SiC Substrate

Epitaxial Graphene

Cross-section TEM of GaN growing between graphene and SiC substrate

Ke Wang, PSU MCL
GaN Intercalation in Epi Graphene

Pathways for Ga intercalation:
Atomic Structure of 2D GaN Layers

Two structurally different 2D layers of GaN at interface:
- Low buckled 2D GaN near graphene
- Highly buckled 2D GaN with nitrogen termination
- Only observed with graphene encapsulation

Ke Wang, PSU MCL
Electronic Structure of 2D GaN Layers

Predicted bandgap energies:
- Low buckled GaN $E_g = 4.96$ eV
- High buckled GaN $E_g = 4.24$ eV
- Composite structure $E_g = 2.02$ eV

Ram Krishna Ghosh and Suman Datta
Summary

- MOCVD is a promising technique for TMDs and layered materials
- Graphene encapsulated MOCVD growth viable method to stabilize 2D GaN
- Future work directed at heterostructure growth, alloys & doping

PSU Collaborators
Dr. Sarah Eichfeld (MRI)
Dr. Josh Robinson (MatSE)
Dr. Nasim Alem (MatSE)
Dr. Suman Datta (EE)
Dr. Ke Wang (MRI)
Dr. Tom Jackson (EE)

Financial support provided by:

Acknowledgements

Graduate Students
Xiaotian Zhang
Zakaria Al Balushi
Nathan Martin
Mel Hainey Jr.

Postdoctoral Scholars
Chen Chen
Jarod Gagnon
Tanushree Choudhury
Wurtzite Bulk Structure of GaN

Materials discovery with computation
Indirect bandgap 4.12 eV

Stabilized Structure

direct bandgap 5.28 eV
The Buckled Structure for 2D III-nitrides is More Stable!
Polarization-induced Topological insulators for memory and quantum computing


Exotic physics

Single-photon emitters for quantum optics and communication
