제 31회 한국반도체학술대회
The 31st Korean Conference on Semiconductors
2024년 1월 24일(수)-26일(금) | 경주화백컨벤션센터(HICO)

광주과학기술원
Gwangju Institute of Science and Technology

# Growth of $HfSe_2$ with *In-situ* BN Passivation for Improved Electrical Properties

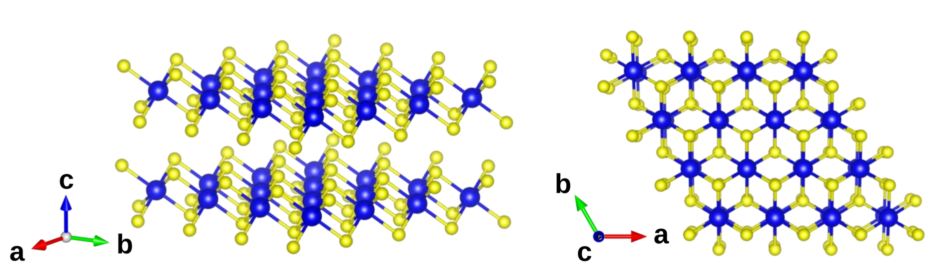

Jung Dae Lee[1] and Sanghan Lee[1]
[1]Gwangju Institute of Science and Technology (GIST), Korea
*E-mail: sanghan@gist.ac.kr


## Abstract


**Hafnium diselenide ($HfSe_2$)** is one of the two-dimensional transition metal dichalcogenides (2D TMD), which maintains very **high electron mobility (~3,500 $cm^2/Vs$) at room temperature** compared to Si (~1,350 $cm^2/Vs$), even when the device channel scale is extremely reduced. However, in previously reported studies, **the mobility of $HfSe_2$ was experimentally very low**, which is considered a major barrier in practical electronic applications. The **very poor air stability of $HfSe_2$**, especially the formation of **selenium blisters** that degrade the surface quality and stoichiometry when exposed to air, is one of the main reasons for its low electron mobility. In this study, we successfully deposited $HfSe_2$ thin films with ***in-situ* boron nitride (BN) passivation** that efficiently prevents the formation of selenium blisters. **Optimized stoichiometry of $HfSe_2$** thin films was achieved by **supplying hafnium metal flux through laser ablation** and **sufficient selenium flux through thermal evaporation**. It was revealed that as-grown $HfSe_2$ thin film has out-of-plane **oriented 1T phase** based on X-ray diffraction (XRD) and Raman spectrum analysis. ***Furthermore, we will investigate its electrical properties through the fabrication of field effect transistors***. We believe that our study will pave the way for the next-generation 2D electronics through follow-up studies.


## 1. Introduction

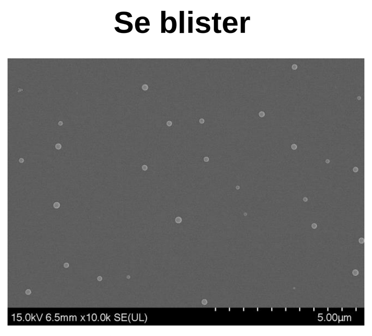
### Low electron mobility of $HfSe_2$




- **Theorical mobility:** 3,579 $cm^2/V\cdot s$
- **Experimental mobility:** 0.22~4 $cm^2/V\cdot s$

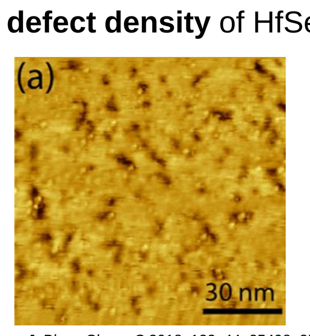
Nano Res. 2014, 7(12): 1731–1737
Sci. Adv. 2017;3:e1700481
Appl. Phys. Lett. 106, 143108 (2015)
Nanoscale, 2017, 9, 1645-1652

**Se blister**



*In preparation*

**High defect density** of $HfSe_2$




J. Phys. Chem. C 2018, 122, 44, 25498–25505

- **A high defect density (black dots)** are observed on exfoliated single crystal $HfSe_2$ surface.
- The **oxidation of $HfSe_2$** formation **insulating $HfO_x$** and **spherical Se blisters are created**.

**Defects** and **oxidation** are considered to **induce scattering**, leading to **low electron mobility.**

### Motivation

**Amorphous boron nitride (a-BN) for passivation**
- **Capping layer** to prevent oxidation of TMD
- **Improvement** of the electrical characteristic of TMD
- **Applicability of PLD methods** to variable material

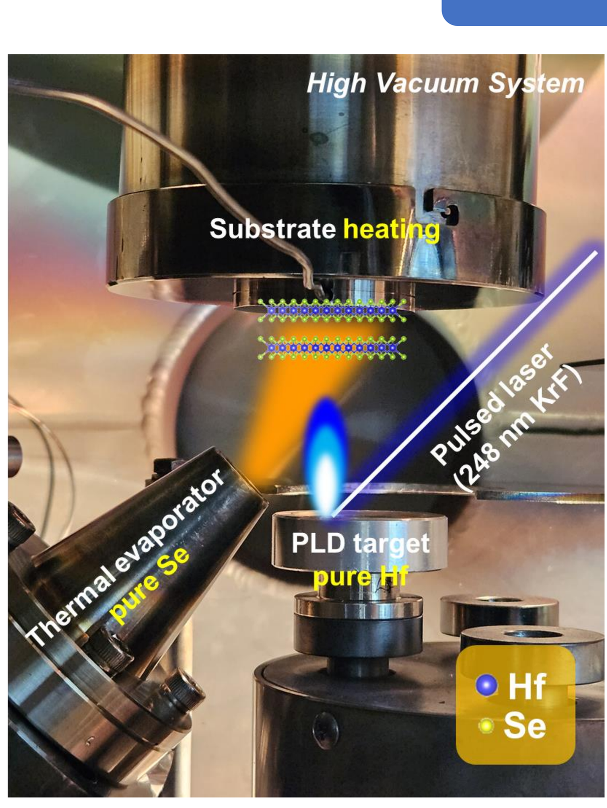
**Recently reported defect engineering**
- The way that control defects is mostly through **post-processing**.
- The approach of defect engineering is **biased toward increasing defects**.

- ***In-situ*** **passivation**
- ***In-situ*** **defect engineering**
- **Defect engineering through a unified approach, whether to increase or decrease**
- **High crystalline** TMD

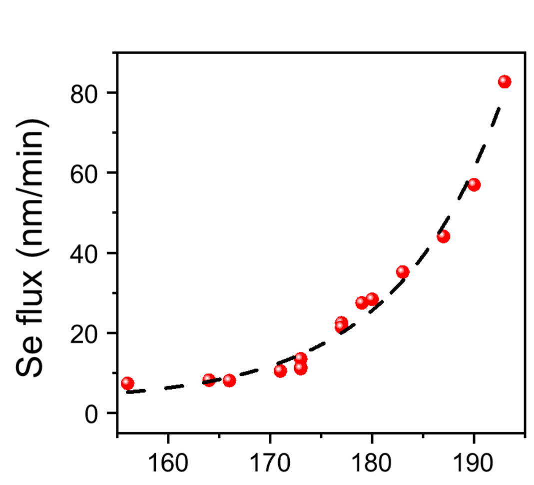
**Hybrid PLD system**

## 2. Methods

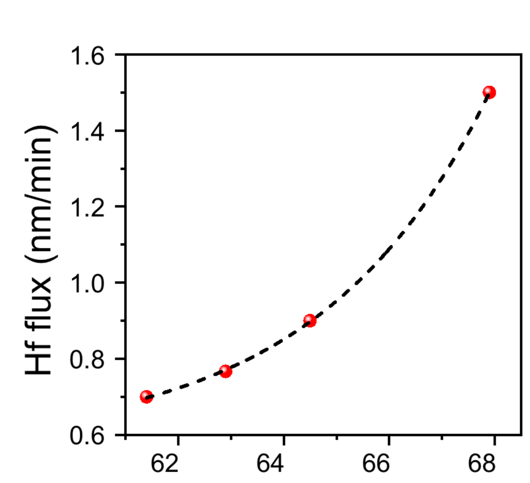
### Hybrid PLD system

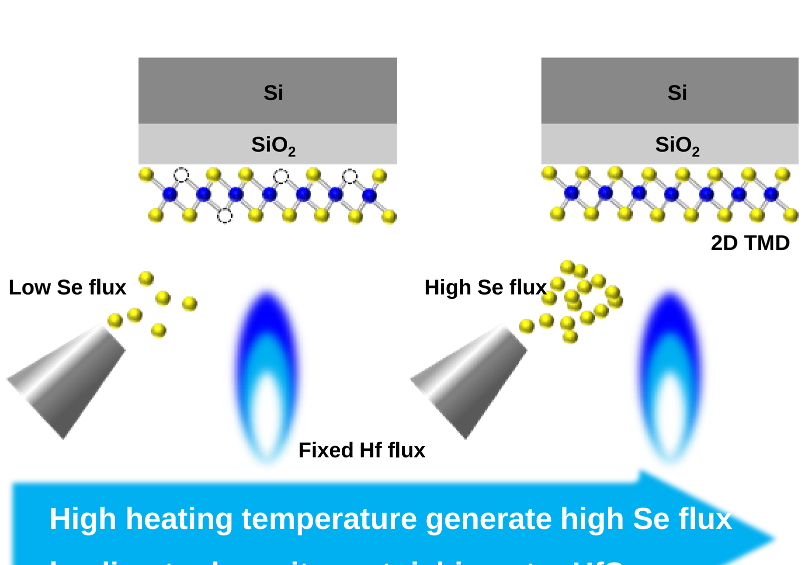



**Thermal Evaporator**
- Dependent on Temperature
- **Temp. ↑ → Se flux up ↑**




**Pulse Laser Deposition**
- Dependent on Laser energy
- **Laser energy ↑ → *Hf flux* ↑**



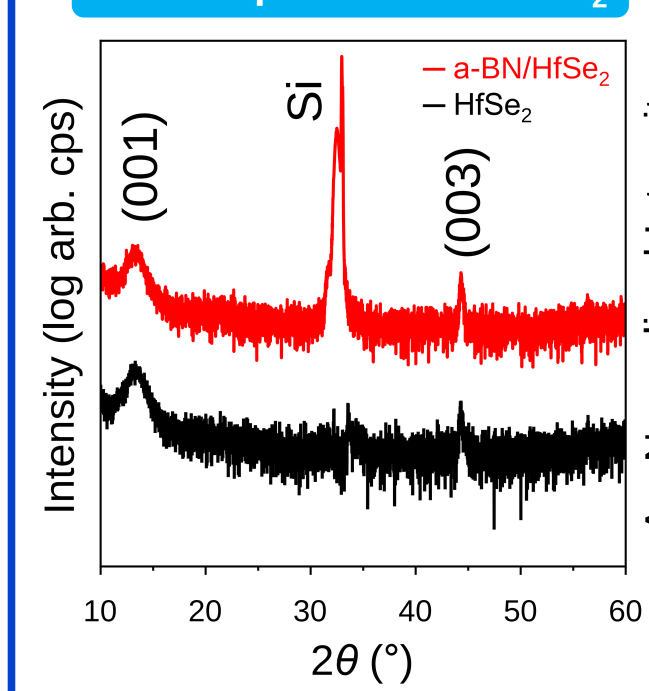



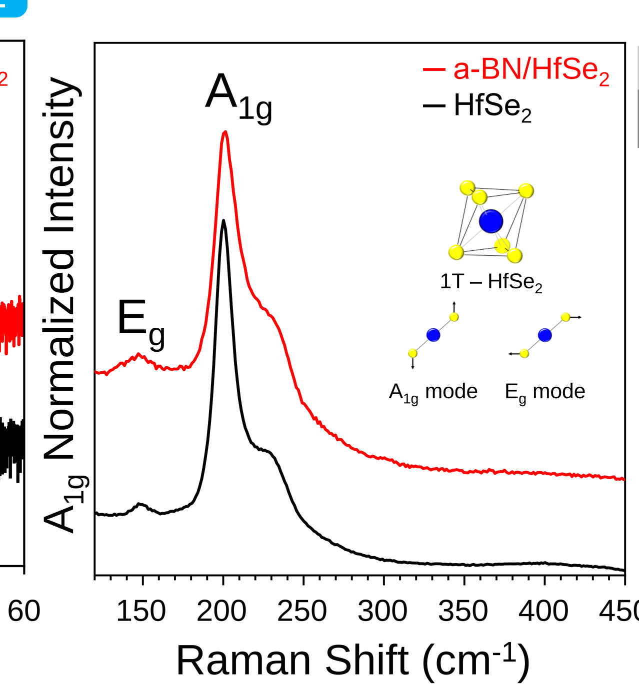

- TMD deposition is driven by **metal flux & Se flux**.
- **The composition of $HfSe_2$ can be controlled** by the Se/Hf flux adjusted the **Se heating temperature**.
- High-quality thin film is deposited using a **single element precursor** in a **high vacuum chamber**.
- PLD chamber can load multiple targets → ***In situ*** **passivation technique** (a-BN) is possible

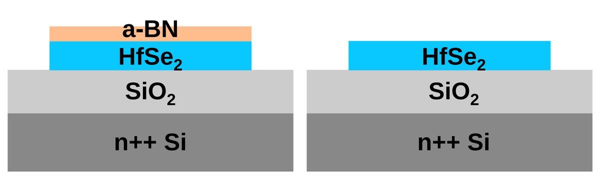
## 3. Results & Discussion

### 3-1) Structural Characterization

**a-BN deposition on $HfSe_2$**



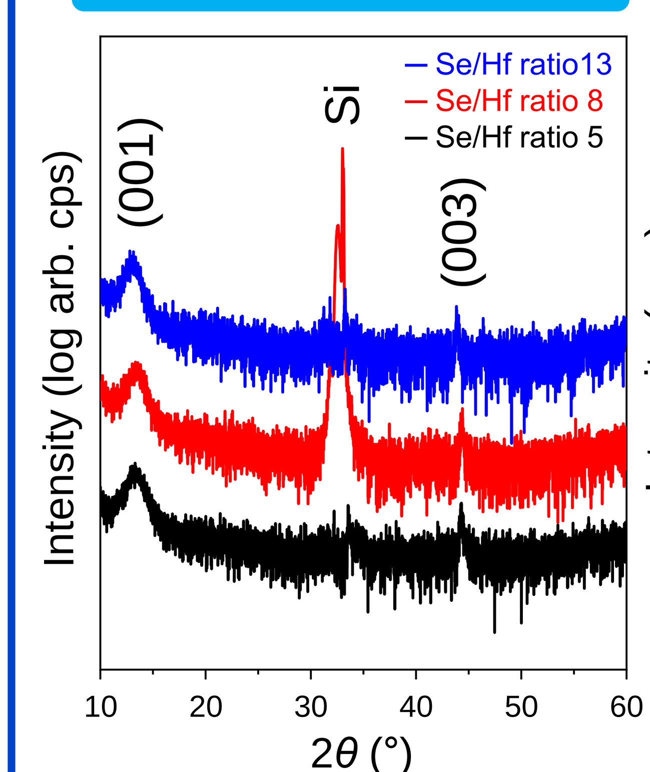



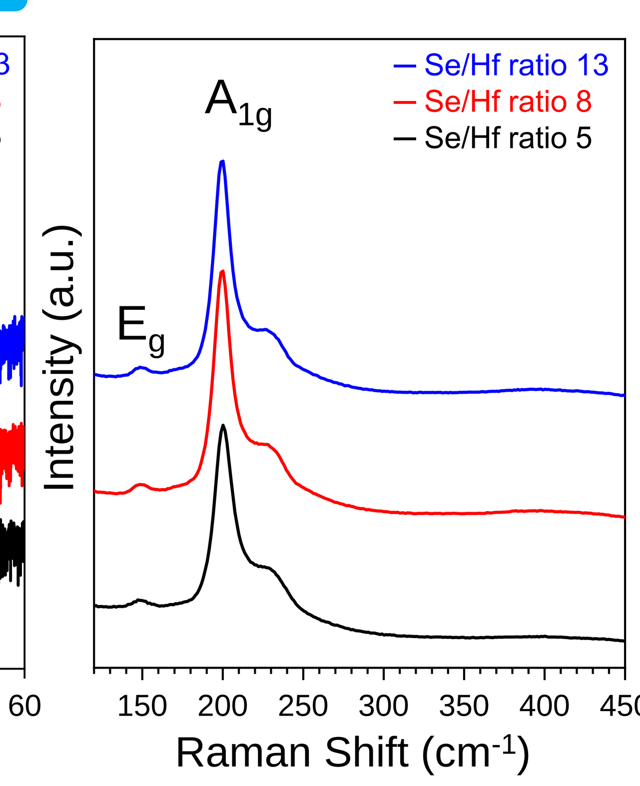




- After a-BN deposition on $HfSe_2$, **crystalline 1T-$HfSe_2$ structure is still observed** through XRD and Raman analysis.

▶ **The a-BN deposition doesn't damage the structure of $HfSe_2$**

**Different Se/Hf flux ratio**

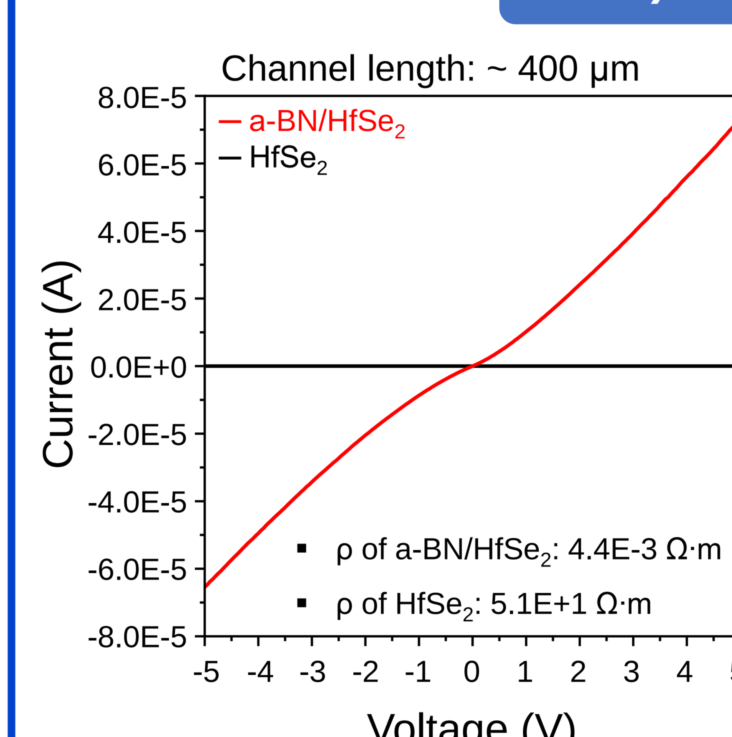


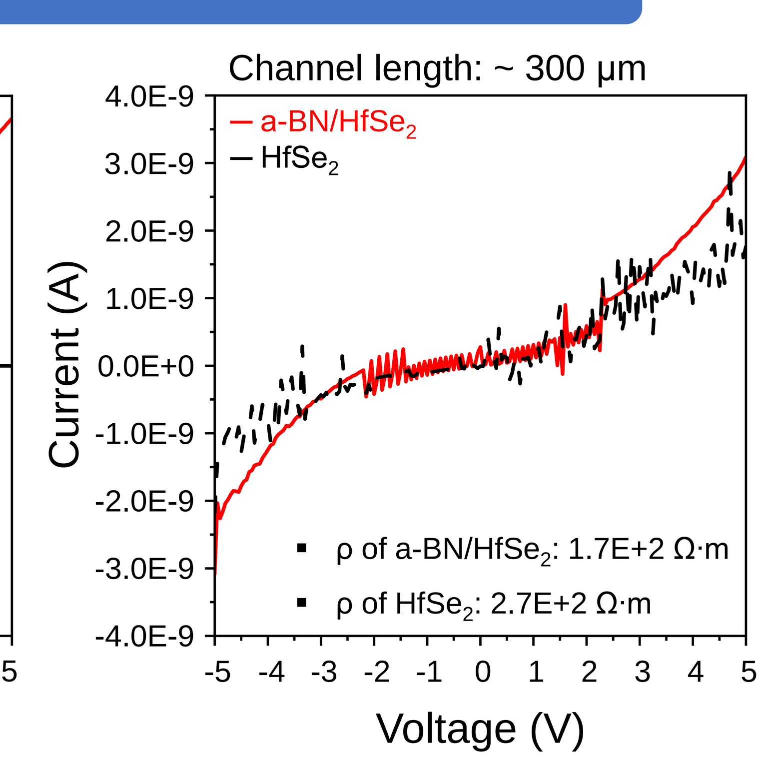



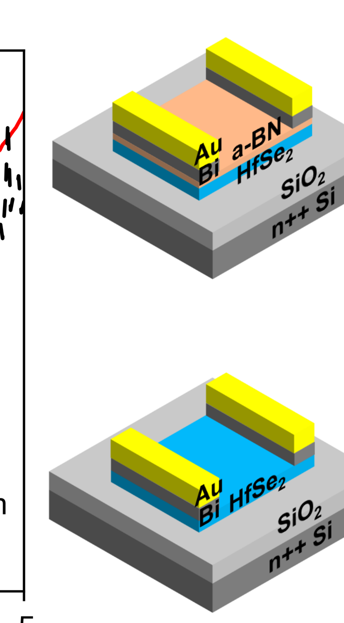

- $HfSe_2$ with the **same 1T phase** is synthesized despite the **different Se/Hf flux ratios**.
- Preferred orientation along **(00*l*) of $HfSe_2$** is **not notably affected by the Se/Hf flux ratio**

▶ **Selenium vacancies can be controlled while maintaining crystallinity and 1T phase**

### 3-2) Electrical Characterization




- **The resistivity** (ρ) **of $HfSe_2$ with a-BN passivation layer was lower** than that of bare $HfSe_2$.

▶ **The a-BN layer is thought to maintain low resistance by preventing the production of insulating $HfO_x$ when $HfSe_2$ is oxidized.**

## 4. Further works

1. **Verifying $HfSe_2$ composition using XPS analysis with variable Se/Hf flux ratio sample**
2. **Developing a fabrication process for $HfSe_2$ channel FET and analyzing the transfer and output curve**
3. **Comparison of device performance of $HfSe_2$ from variable Se/Hf flux ratio**
4. **Assessing the passivation effect by aging test and checking the formation of Se blister between a-BN/$HfSe_2$ and bare $HfSe_2$**

## 5. Conclusion

1. **The hybrid PLD system demonstrates the capability to deposit crystalline 1T-$HfSe_2$ on Si while varying Se/Hf flux ratios.**
2. **Deposition of the a-BN layer *via* PLD does not damage the crystalline 1T-$HfSe_2$ structure, allowing *in situ* passivation in this system.**
3. **Analyzing the resistivity of a-BN/$HfSe_2$ and $HfSe_2$, the a-BN layer is considered to act as a passivation layer, preventing the formation of insulating $HfO_x$.**

SEED
Sustainable Energy and Electronic Devices laboratory