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# Molecular Beam Epitaxy of TaSe<sub>2</sub> on GaP(111)B

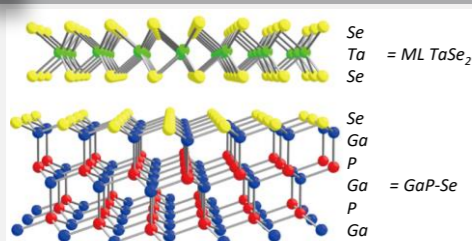
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## Context and goal



Transition-Metal Dichalcogenides (TMDCs) are 2D materials made of layers of a transition metal covalently bonded to atomic planes of chalcogens (S, Se, Te).

This study focus on TaSe<sub>2</sub>, which has two polymorphs with different properties.

- 1T-TaSe<sub>2</sub>, with octahedral coordination, forms a Charge Density Waves (CDW) at room temperature and is a Mott insulator in few monolayers.
- 2H-TaSe<sub>2</sub>, with hexagonal coordination, is metallic and could be used in combination with other TMDC to form appropriate contacts.

Molecular Beam Epitaxy (MBE) of TaSe<sub>2</sub> has been reported via van der Waals (vdW) epitaxy on graphene and pseudo vdW on Se-terminated GaAs and AlN.

We present MBE growth on Se-terminated GaP, a substrate that has the following advantages:

- small lattice mismatch with Si
- higher thermal stability than GaAs

[1] A. Ohtake et al. "Evolution of surface and interface structures in molecular-beam epitaxy of MoSe<sub>2</sub> on GaAs (111) A and (111) B", *Crystal Growth & Design* 17.1 (2017), pp. 363–367

## Influence of growth conditions

### Sample preparation

Preparation of GaP(111)B-Se:

(a) GaP(111)B substrates are deoxidized under PH<sub>3</sub> and atomic H in a III-V MBE reactor and exhibit a 2x2 reconstruction

(b) GaP-Se terminated are prepared under a Se flux in the 10<sup>-4</sup>T range from 250°C to 450°C in a TMDC reactor

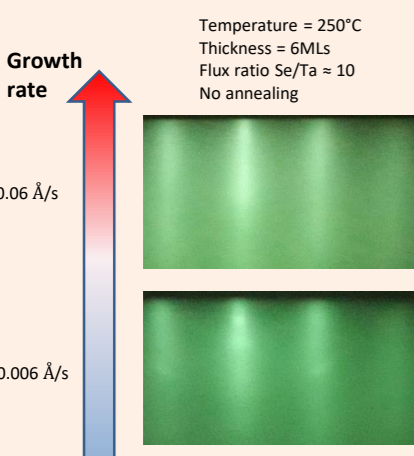


TaSe<sub>2</sub> growth:

- Growth temperature from 250 to 650°C
- Typical Ta growth rate between 0.001 and 0.02 Å/s
- Se flux ranging from 10<sup>-7</sup> to 10<sup>-5</sup> Torr
- Annealing under Se flux up to 750°C

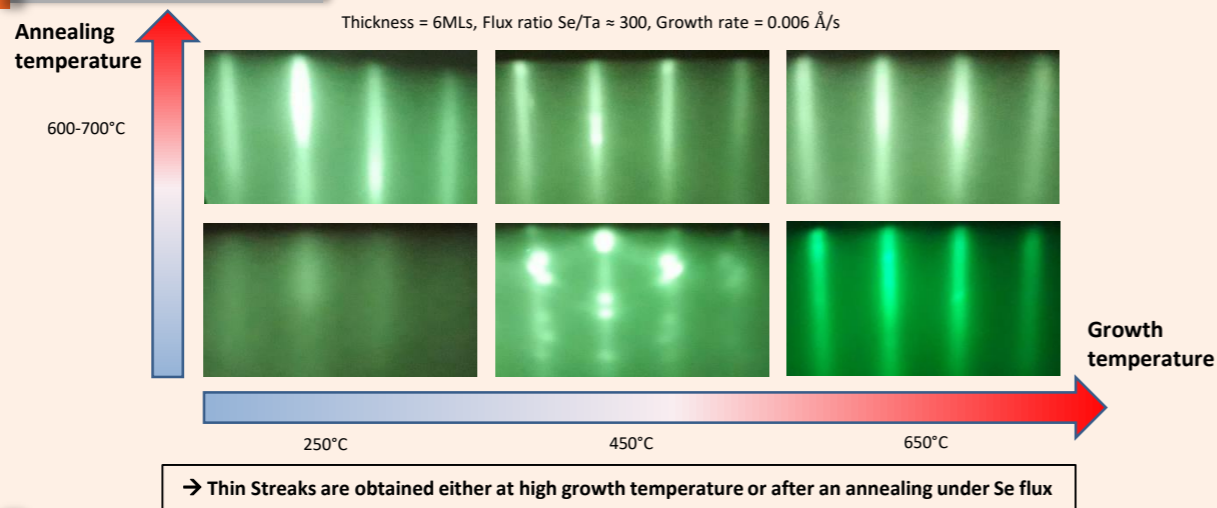
Se capping layer (30-50 nm) for ex-situ characterizations (XRD, STM)

### Growth rate

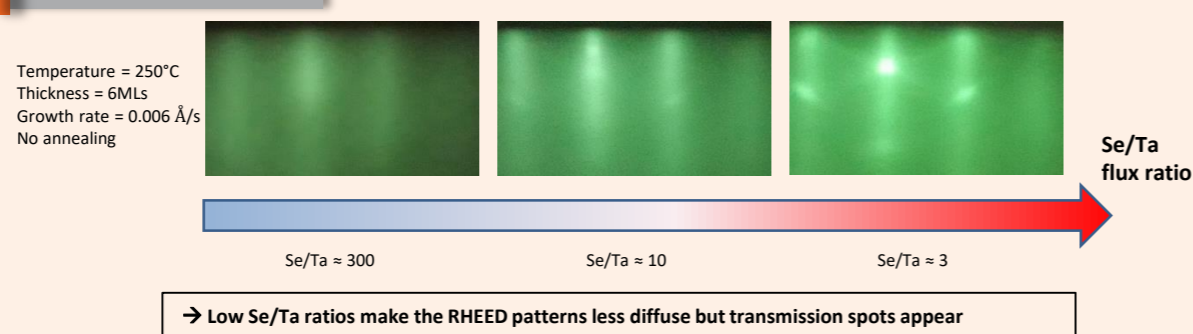


→ No influence of the growth rate at 250°C

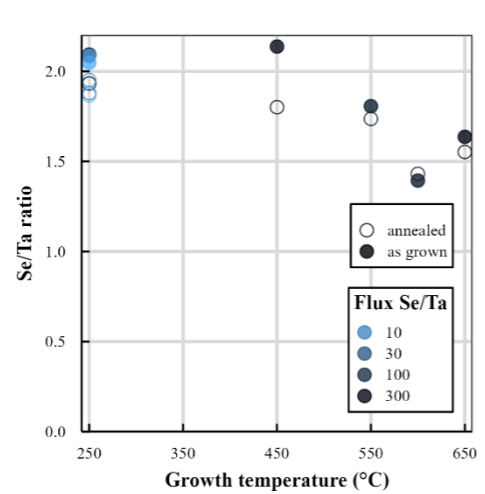
### Temperature



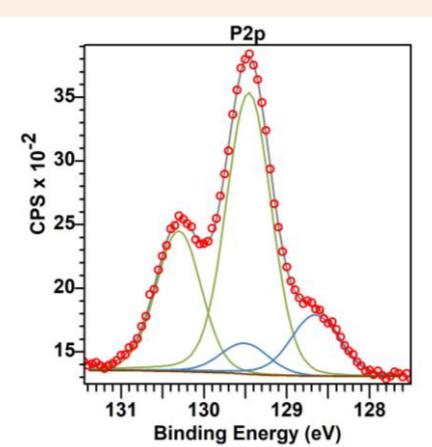
### Se/Ta flux ratio



### High temperature degradations



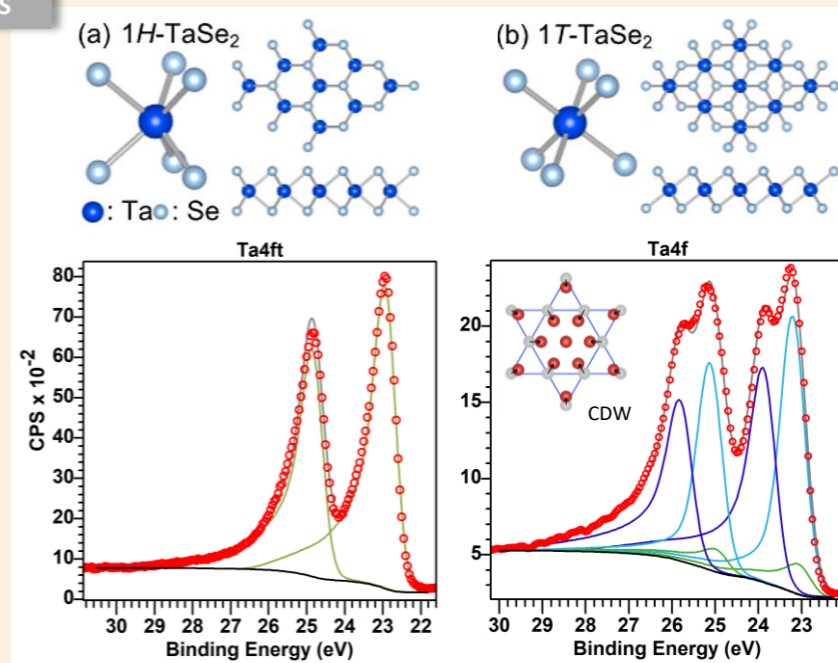
▲ Se/Ta ratios calculated from XPS



→ Decrease of the Se/Ta ratio at high temperature  
→ Little influence of the flux ratio on the Se/Ta ratio  
→ Appearance of a new P 2p component (possibly Ta-P bonds) at high growth or annealing temperature

## Phase determination

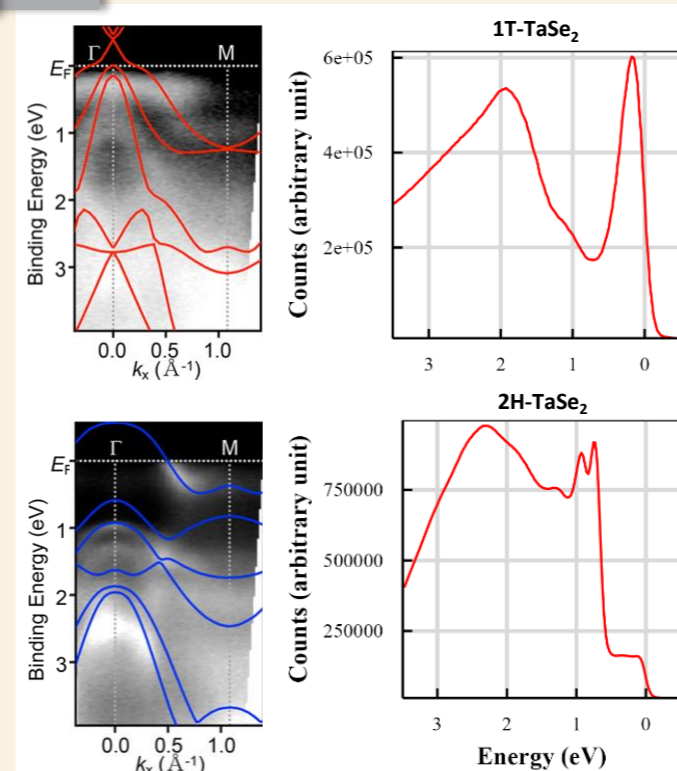
XPS



◀ Crystal structure of (a) 1H and (b) 1T phases of TaSe<sub>2</sub> [2]

◀ Corresponding Ta4f lines measured in XPS (Al K<sub>α</sub>), inset schematic from [3]

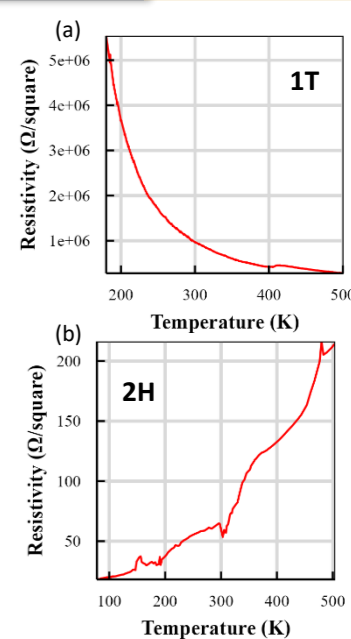
UPS



◀ Band structure calculations and measurements from [2], UPS spectra (He I) around  $\Gamma$  of 1ML 1T-TaSe<sub>2</sub> grown at 550°C and 6ML 2H-TaSe<sub>2</sub> grown at 250°C and annealed at 700°C

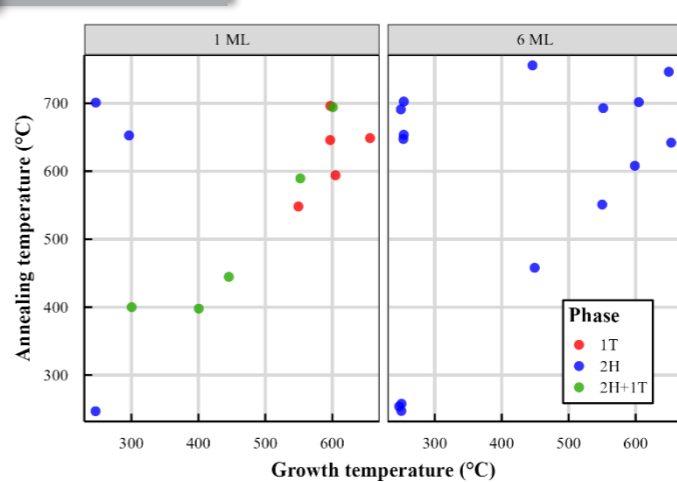
→ Despite being an insulator, 1ML 1T-TaSe<sub>2</sub> has an important electron density at E<sub>v</sub> around  $\Gamma$ .  
→ On the other hand 2H-TaSe<sub>2</sub> has its first valence bands at 0.8 and 1 eV

### Resistivity



▲ Electrical resistivity of (a) 1T-TaSe<sub>2</sub> 1ML and (b) 2H-TaSe<sub>2</sub> 6MLs, measured as function of temperature using the four-point method

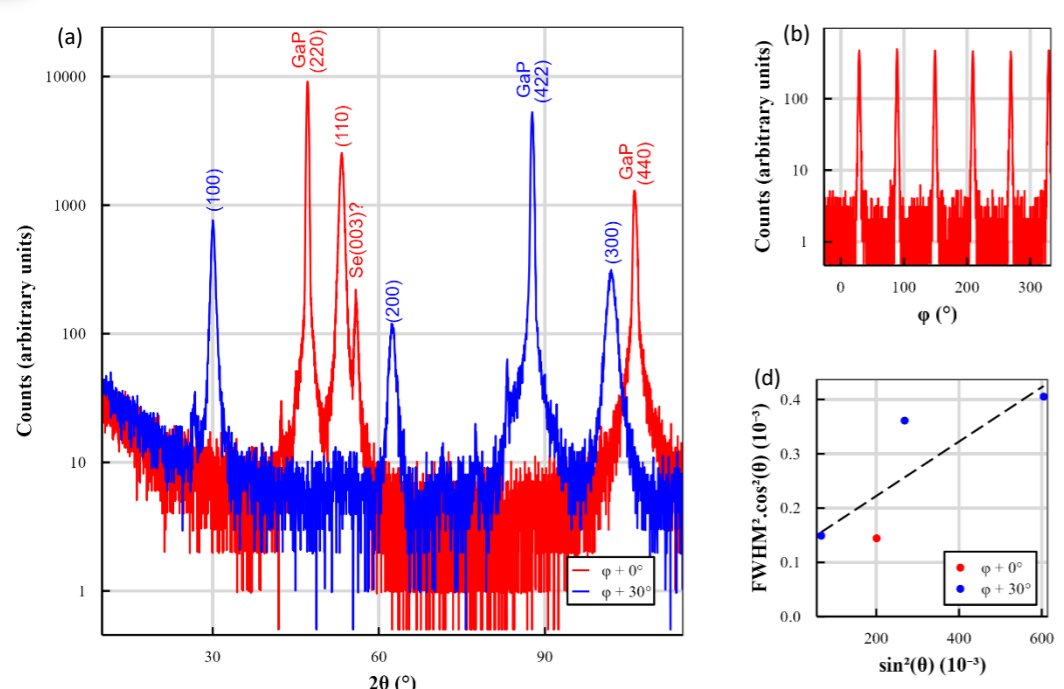
### Obtained phases



→ 1T-TaSe<sub>2</sub> is obtained at high temperature in monolayer  
→ 2H-TaSe<sub>2</sub> is formed in multilayer independently of growth conditions  
→ 1T-TaSe<sub>2</sub> tends to convert into 2H-TaSe<sub>2</sub> upon annealing

[2] Y. Nakata, et al., "Selective fabrication of Mott-insulating and metallic monolayer TaSe<sub>2</sub>", *ACS Applied Nano Materials* 1.4 (2018), pp. 1456–1460.  
[3] Y. Nakata et al., "Robust charge-density wave strengthened by electron correlations in monolayer 1T-TaSe<sub>2</sub> and 1T-NbSe<sub>2</sub>", *Nat Commun* 12 (2021), p. 5873

## XRD analysis of 6MLs 2H-TaSe<sub>2</sub>



→ TaSe<sub>2</sub> well oriented along GaP directions :  
TaSe<sub>2</sub> [0001] // GaP (111)  
TaSe<sub>2</sub> [10-10] // GaP (-211)

$$\beta_m^2 = \beta_{instr}^2 + \beta_{size}^2 + \beta_{strain}^2$$

$$\beta_m^2 - \beta_{instr}^2 = (4\epsilon \tan \theta)^2 + \left(\frac{k\lambda}{\cos \theta}\right)^2$$

$$(\beta_m^2 - \beta_{instr}^2) \cos^2 \theta = (4\epsilon)^2 \sin^2 \theta + \left(\frac{k\lambda}{\cos \theta}\right)^2$$

→ Broadening due to both crystallite size and strain (defects)  
→ Crystallite size = 12 nm

## AFM, STM and LEED imaging of 1ML 1T-TaSe<sub>2</sub>

