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

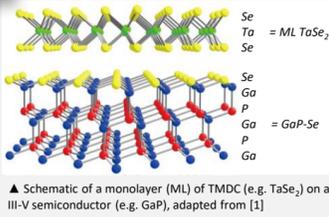
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## Context and goal



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

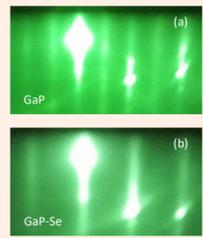
## Influence of growth conditions

### 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

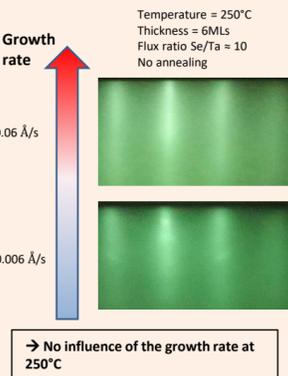


TaSe<sub>2</sub> growth:

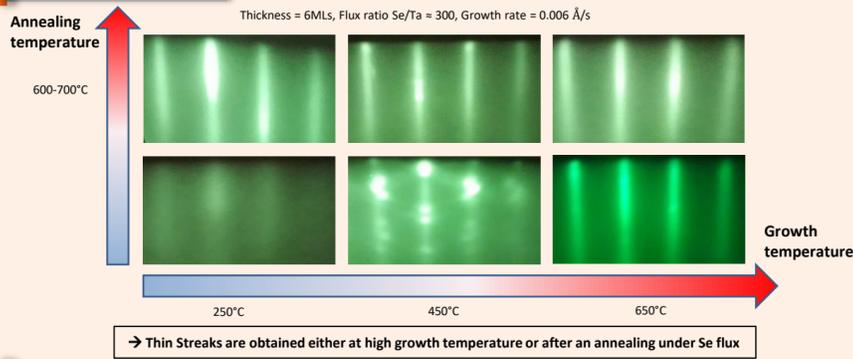
- Growth temperature from 250 to 650°C
- Typical Ta growth rate between 0.001 and 0.02 Å/s
- Se flux ranging from 10<sup>-7</sup> to 10<sup>-5</sup> Torr
- Annealing under Se flux up to 750°C

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

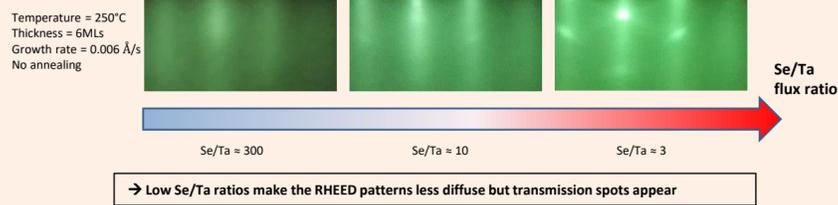
### Growth rate



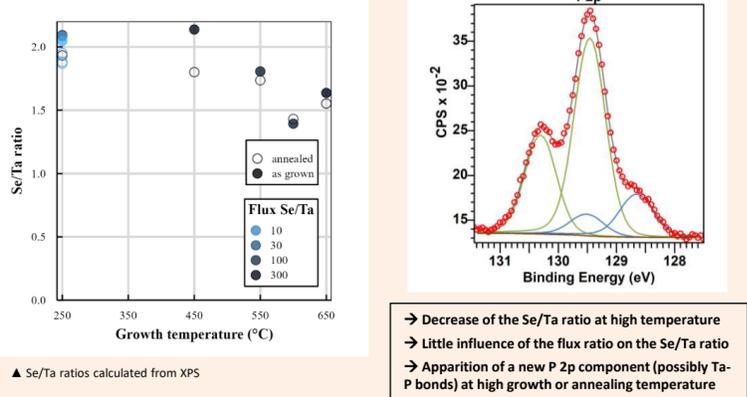
### Temperature



### Se/Ta flux ratio



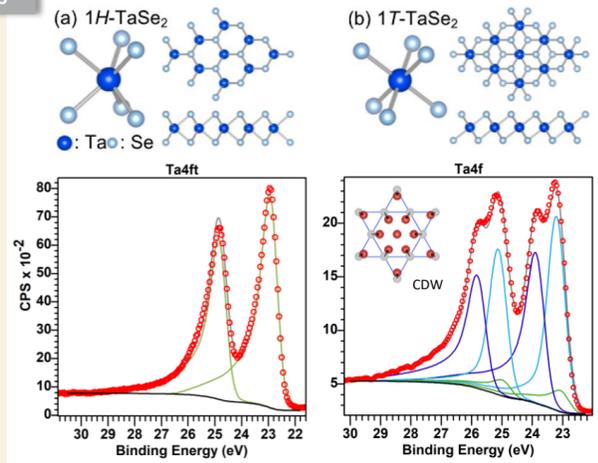
### High temperature degradations



▲ Se/Ta ratios calculated from XPS

## Phase determination

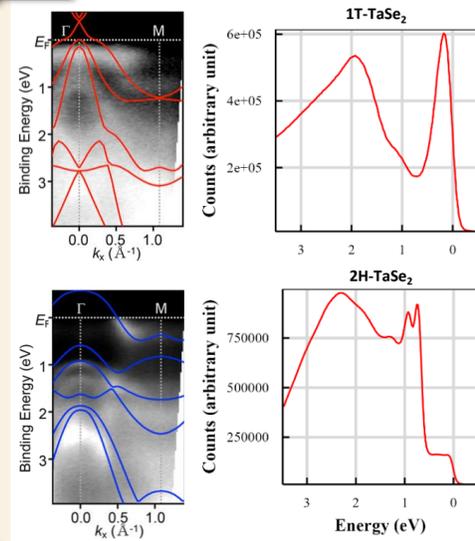
XPS



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

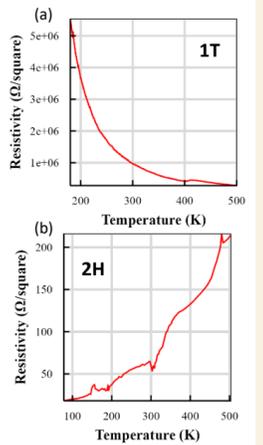
◀ Corresponding Ta4f lines measured in XPS (Al K<sub>α</sub>), inset schematic from [3]

UPS

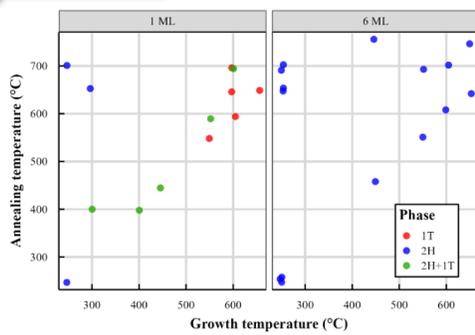


◀ Band structure calculations and measurements from [2], UPS spectra (He I) around Γ of 1ML 1T-TaSe<sub>2</sub> grown at 550°C and 6ML 2H-TaSe<sub>2</sub> grown at 250°C and annealed at 700°C

### Resistivity

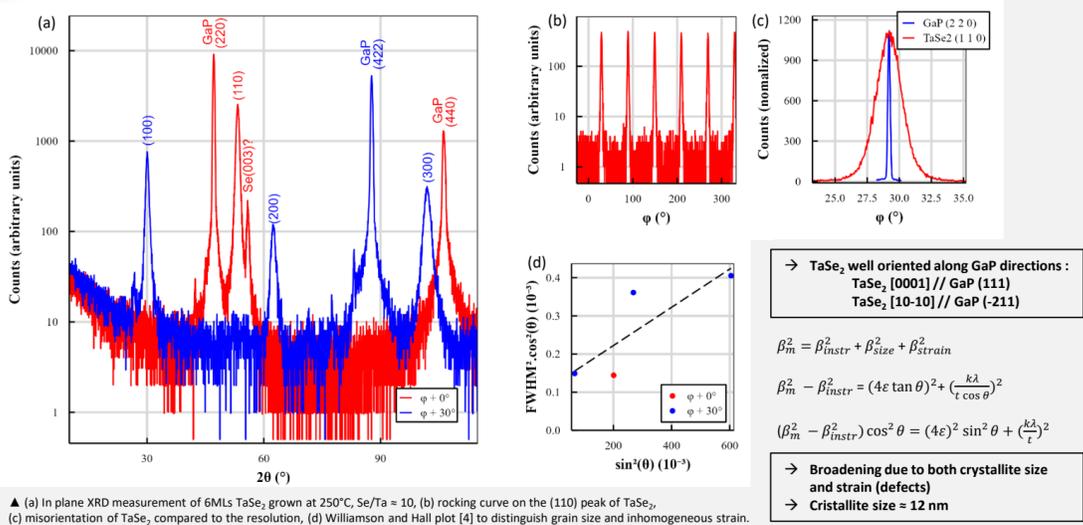


### Obtained phases



[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>



[4] G. K. Williamson et al., "X-ray line broadening from filed aluminium and wolfram", *Acta Metallurgica* 1:1 (1953), pp. 22–31, 0001-6160

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

