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Molecular Beam Epitaxy of TaSe₂ on GaP(111)B

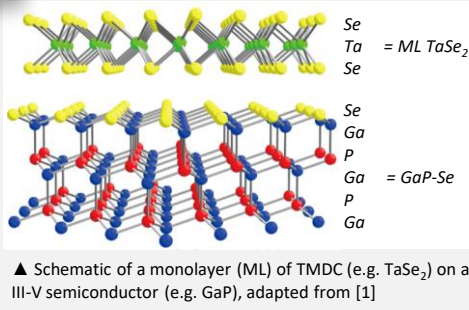
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Context and goal



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 TaSe₂, which has two polymorphs with different properties.

- 1T-TaSe₂, with octahedral coordination, forms a Charge Density Waves (CDW) at room temperature and is a Mott insulator in few monolayers.
- 2H-TaSe₂, with hexagonal coordination, is metallic and could be used in combination with other TMDC to form appropriate contacts.

Molecular Beam Epitaxy (MBE) of TaSe₂ 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 MoSe₂ on GaAs (111) A and (111) B", *Crystal Growth & Design* 17.1 (2017), pp. 363–367

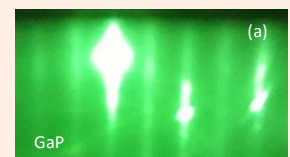
Influence of growth conditions

Sample preparation

Preparation of GaP(111)B-Se:

(a) GaP(111)B substrates are deoxidized under PH₃ 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 10⁻⁴T range from 250°C to 450°C in a TMDC reactor

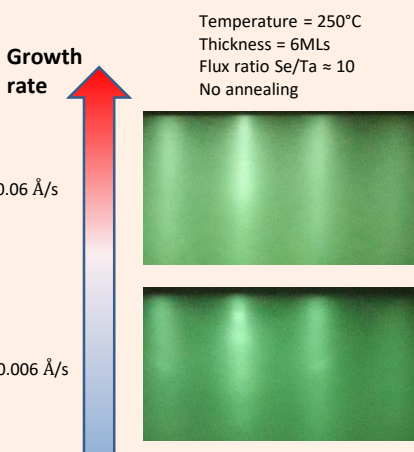


TaSe₂ growth:

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

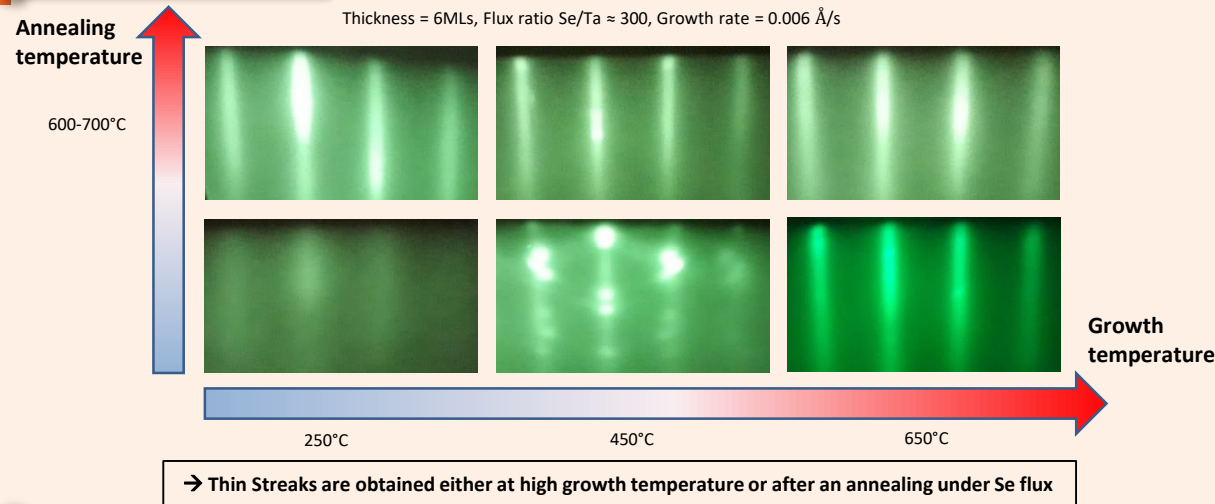
Se capping layer (30-50 nm) for ex-situ characterizations (XRD, STM)

Growth rate

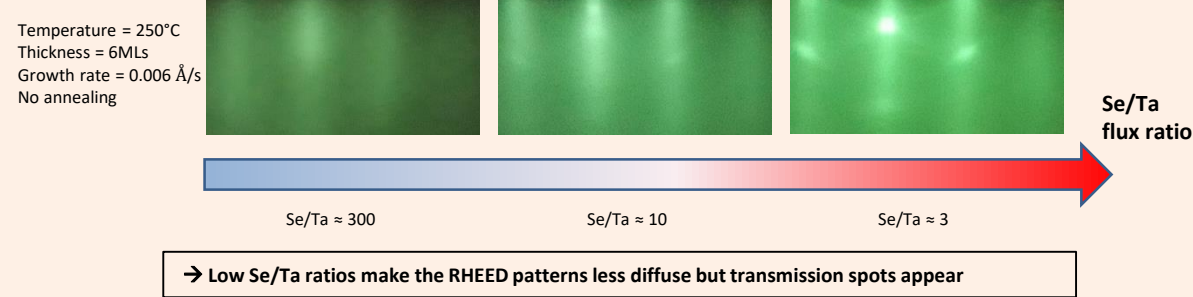


→ No influence of the growth rate at 250°C

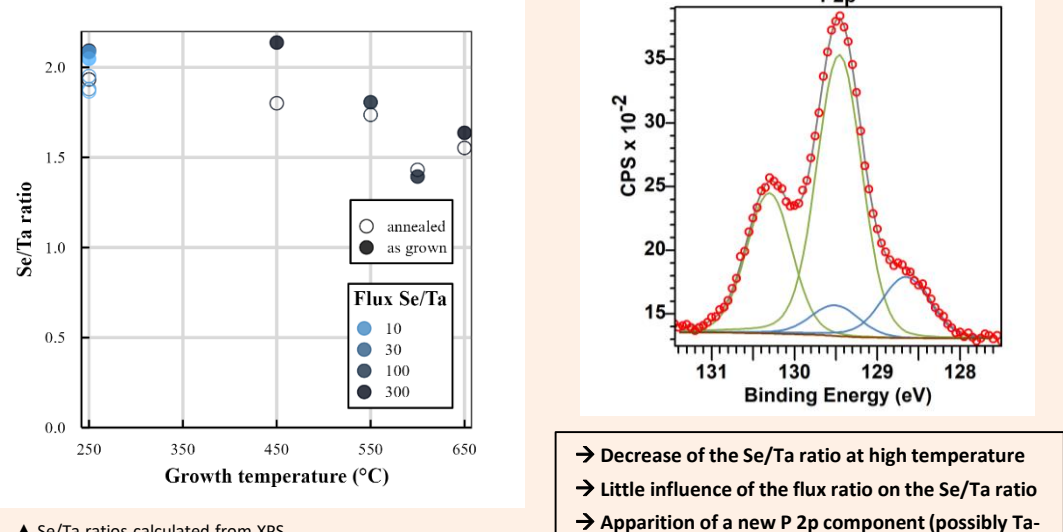
Temperature



Se/Ta flux ratio



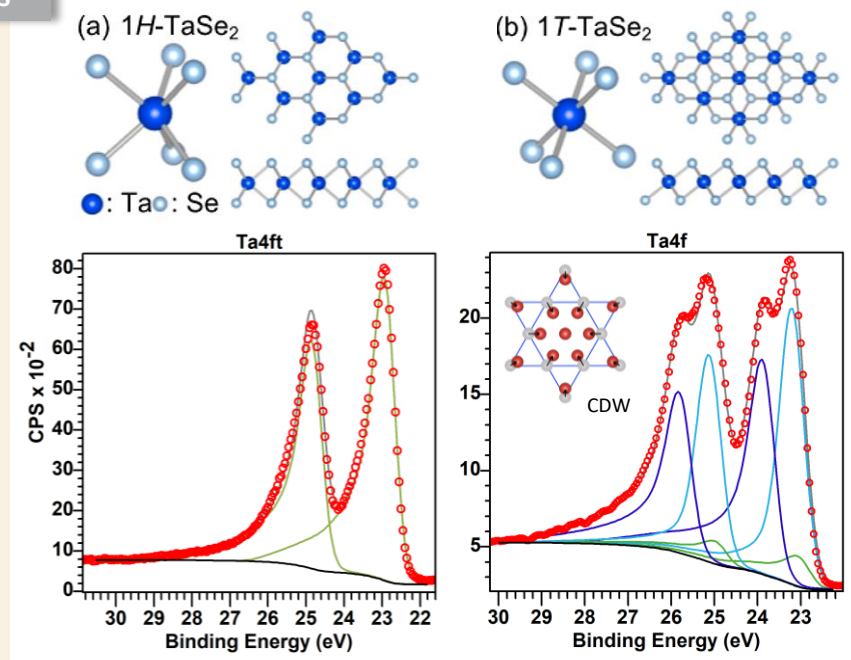
High temperature degradations



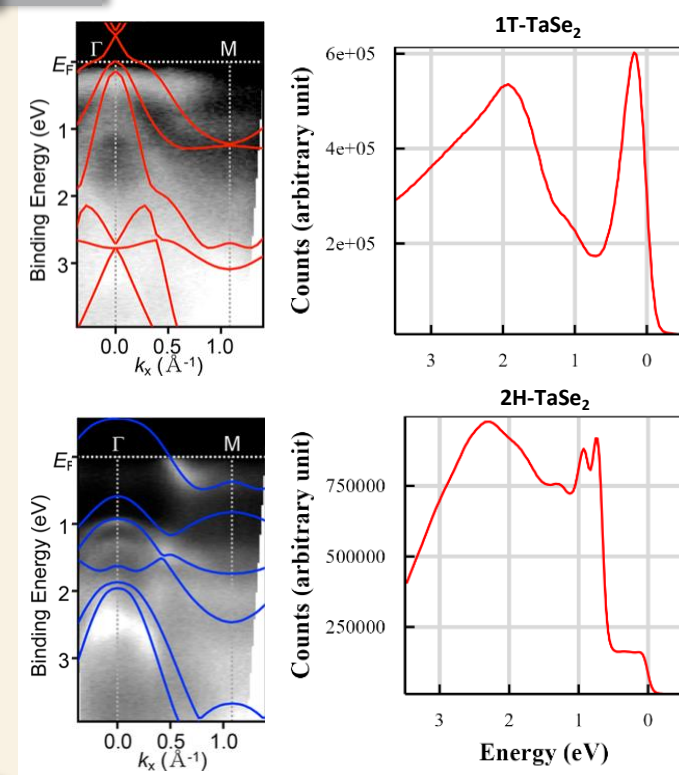
▲ Se/Ta ratios calculated from XPS

Phase determination

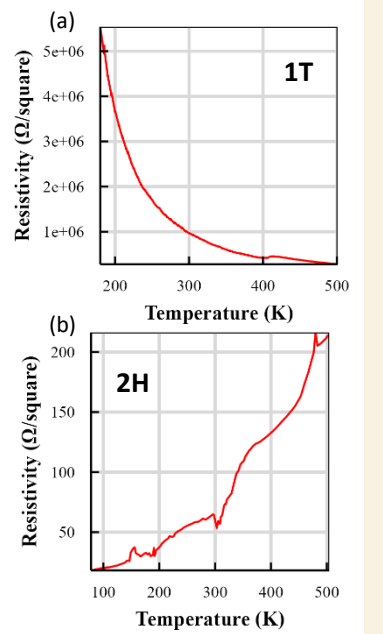
XPS



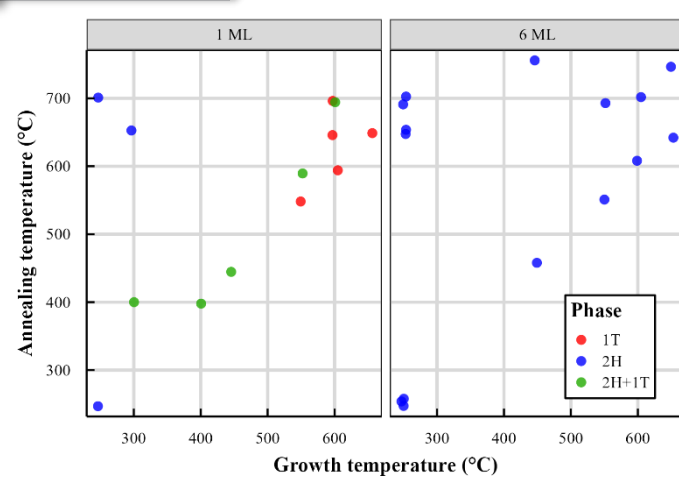
UPS



Resistivity



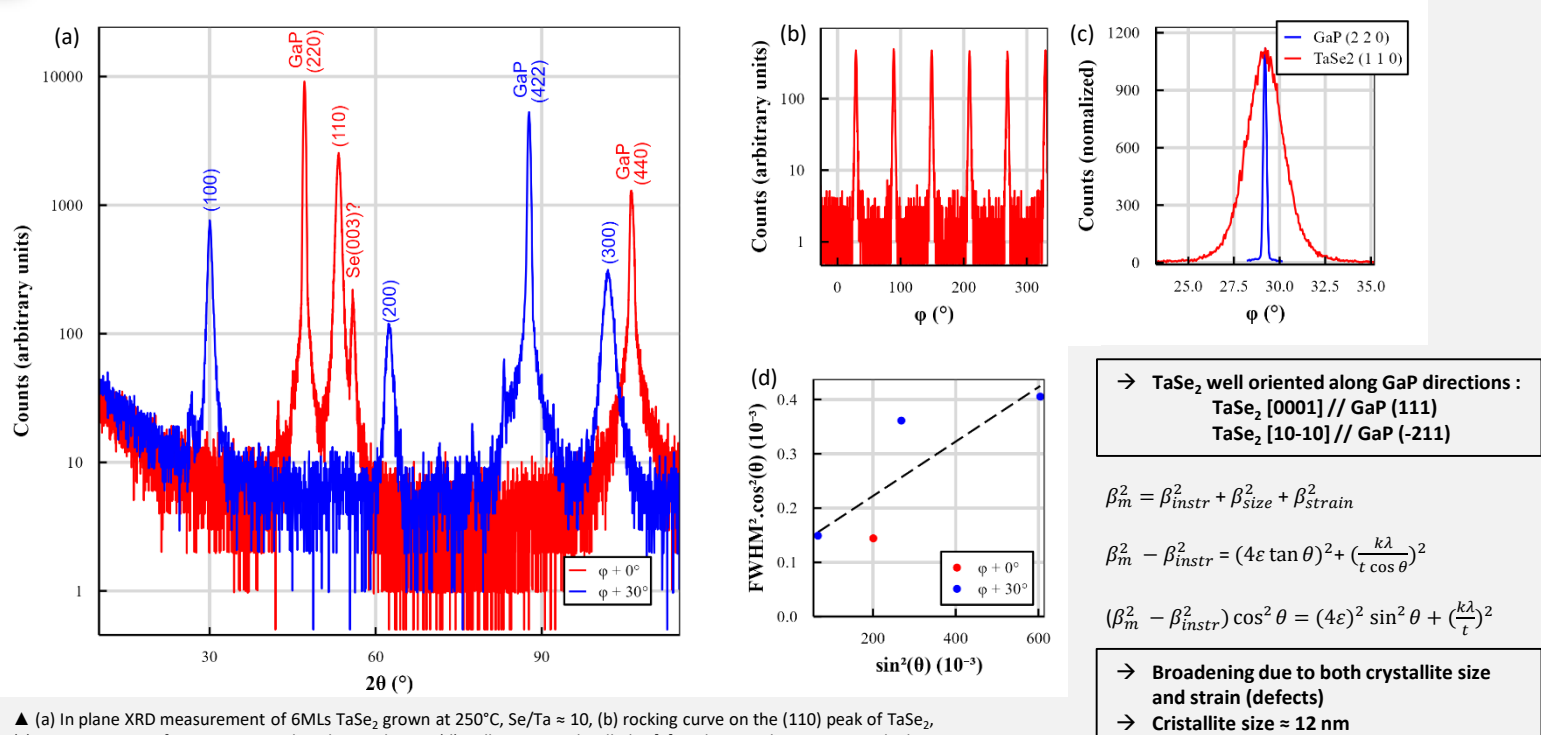
Obtained phases



[2] Y. Nakata, et al. "Selective fabrication of Mott-insulating and metallic monolayer TaSe₂", *ACS Applied Nano Materials* 1.4 (2018), pp. 1456–1460.

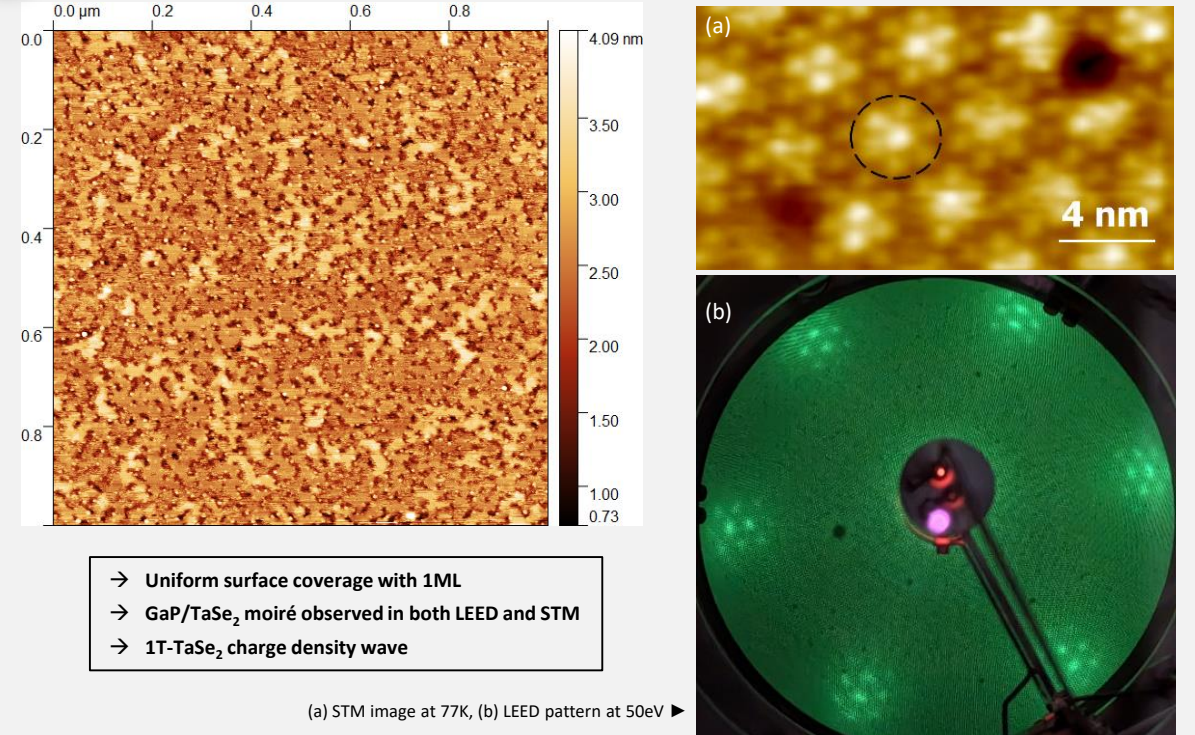
[3] Y. Nakata et al., "Robust charge-density wave strengthened by electron correlations in monolayer 1T-TaSe₂ and 1T-NbSe₂", *Nat Commun* 12 (2021), p. 5873

XRD analysis of 6MLs 2H-TaSe₂



[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-TaSe₂



(a) STM image at 77K, (b) LEED pattern at 50eV