SIMPLANT:
Synthesis of few layered transition metal dichalcogenides by ion implantation

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Laboratory of Solid State Physics and Magnetism, KU Leuven

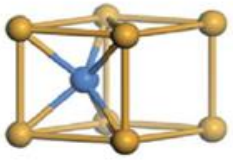
Quick overview

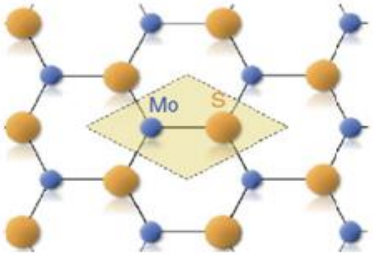
Objective: develop a novel method for the industrial synthesis of TMDCs

Call FLAG-ERA 2017

- Duration: 24 mois;
- ~ 850 k€ total funding.
- 5 parters:
  - LPICM, CNRS-Ecole polytechnique (France), coordinator,
  - TRT (France),
  - Fritz Haber Institute (Berlin, Germany),
  - Institute for Nuclear and Radiation Physics, KU Leuven (Belgium),
  - Laboratory of Solid State Physics and Magnetism, KU Leuven (Belgium).

Basic idea:





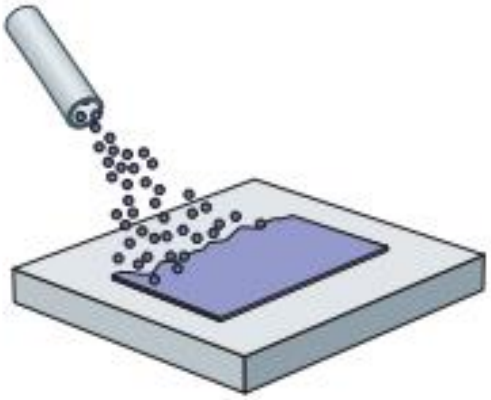
2D materials :
a few 10^{15} Atomes/cm^2

Ex: MoS_2: 1.16 and 2.32 x 10^{15}/cm^2 for Mo and S atoms respectively.

➡ Easily accessible by ion implatation

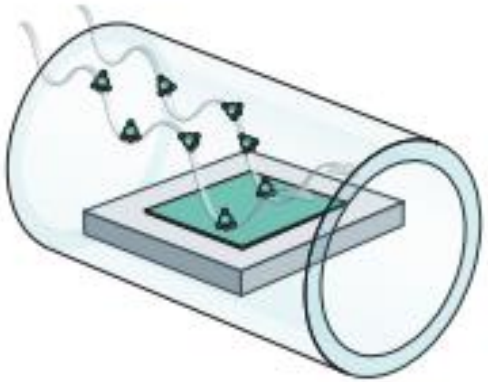
Major synthesis techniques for TMDCs

a Micromechanical exfoliation



b Physical vapour deposition

MBE,
Sputtering,

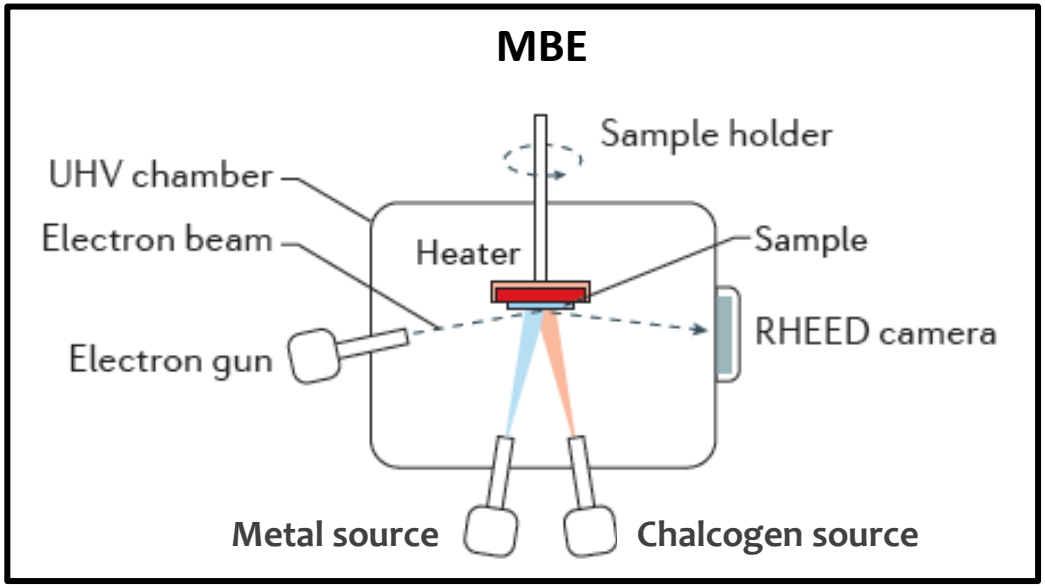


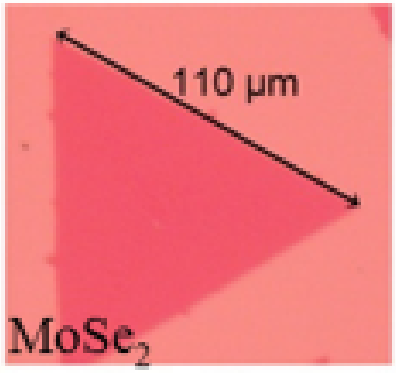
c Chemical vapour deposition

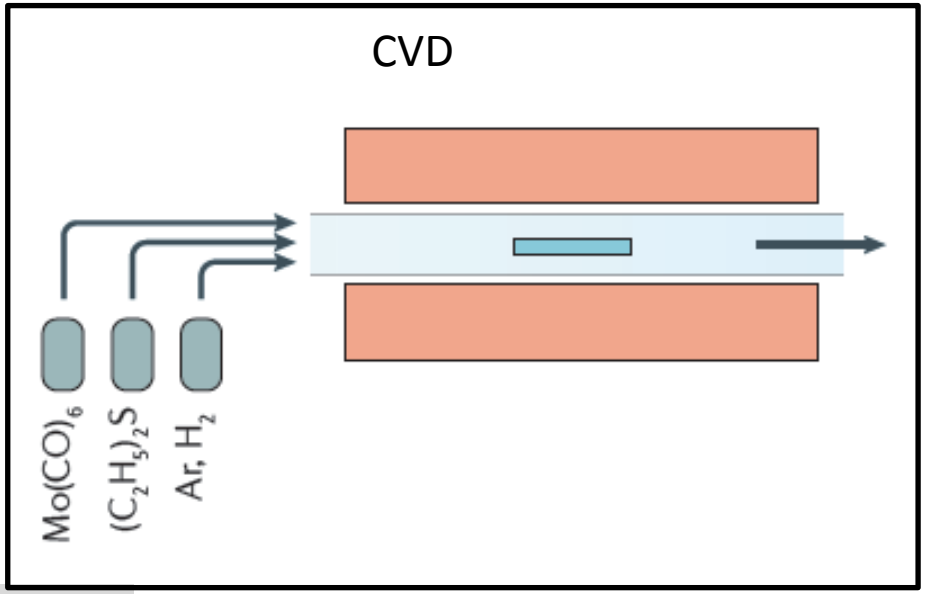
CVD,
ALD,
VPT.

Mannix, *Nature Rev. Chemistry*, **1**, 0014 (2017)

MBE and CVD growth of TMDCs

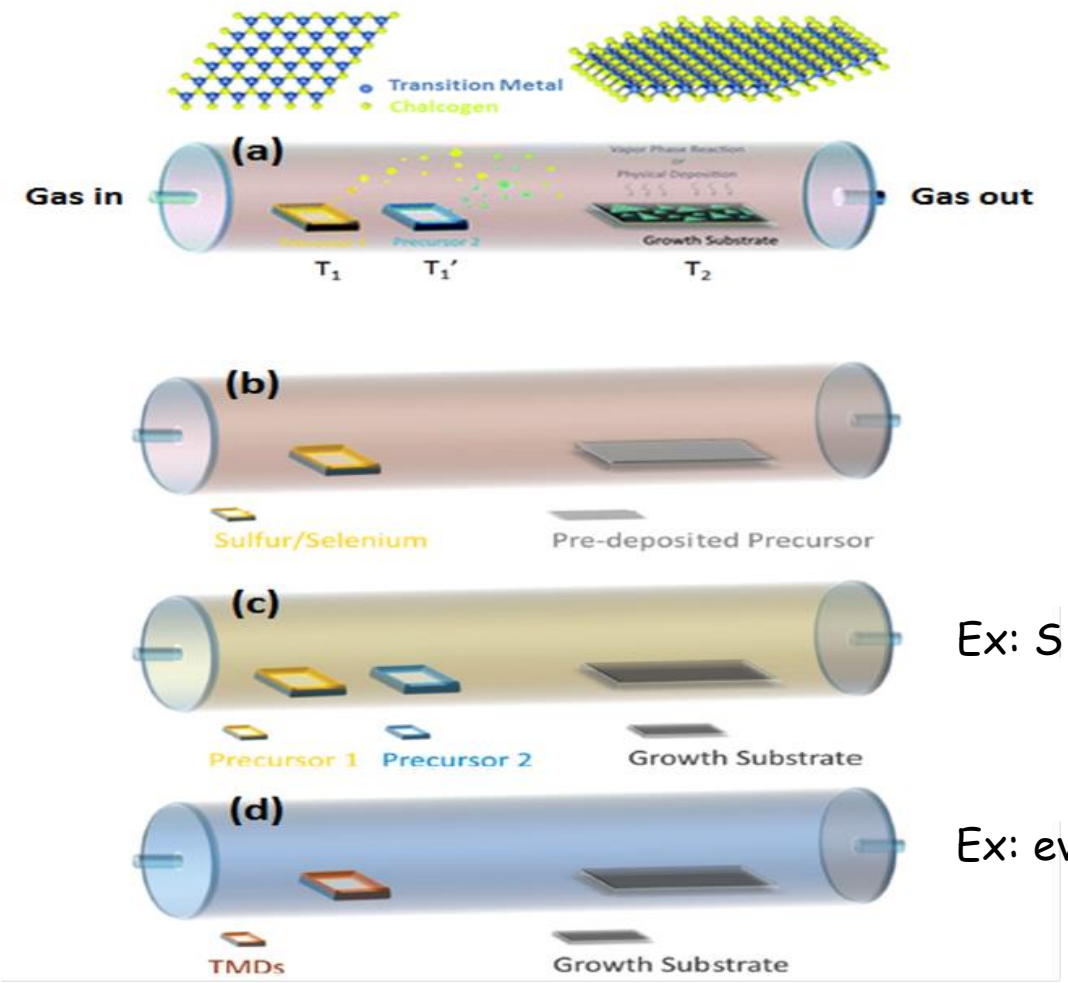






Dong & Kuljanishvili, *J. Vac. Sci. Technol*., **B 35**, 030803 (2017)

Vapour phase transport



Ex: S et MoO_3

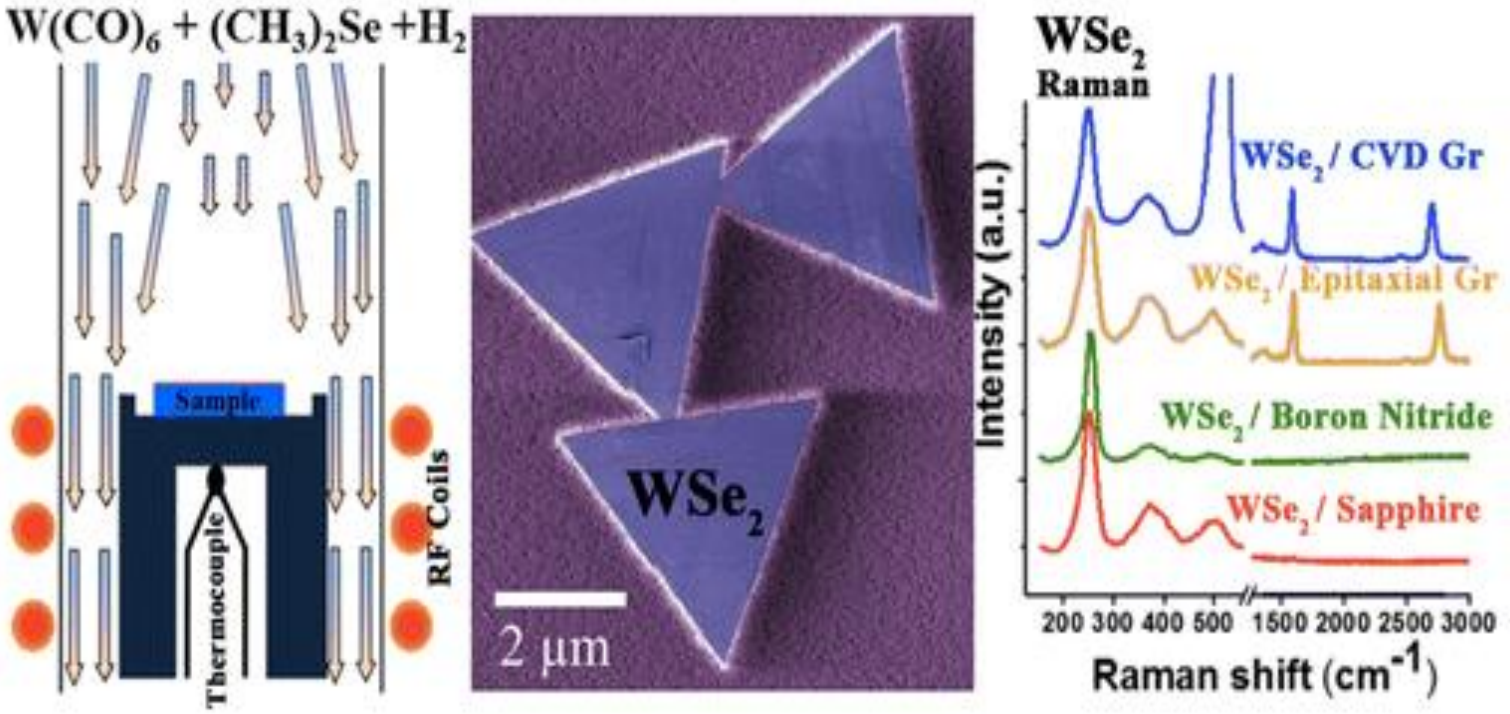
Ex: evap MoS_2 à ~ 900°C

Also direct decomposition of $(NH4)_2MoS_4$

Bosi, *RSC Adv.*, **5**, 75500 (2015)

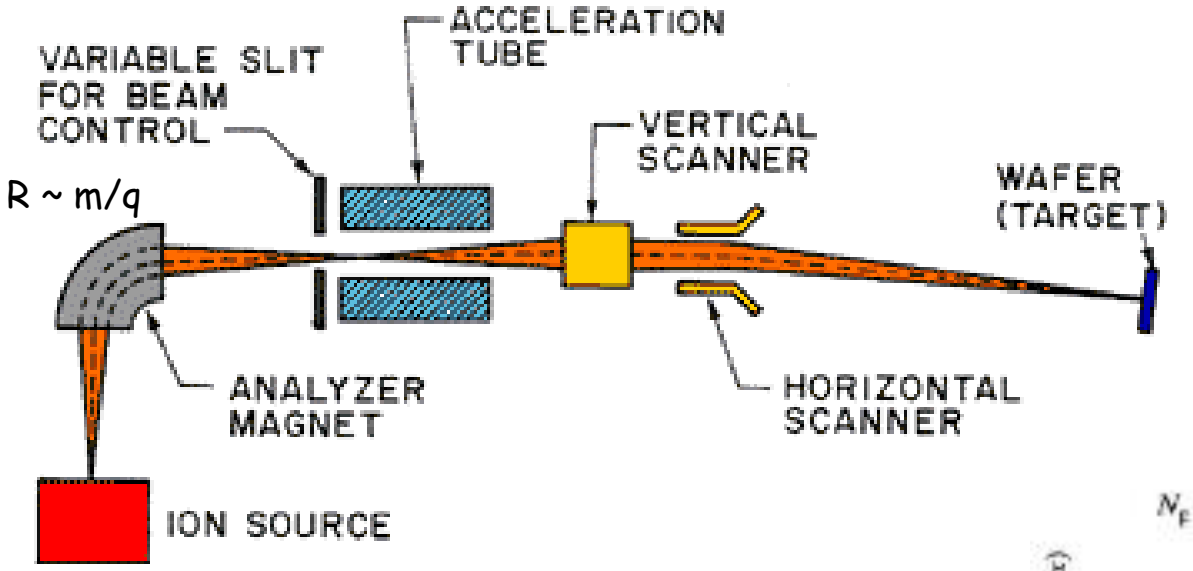
Non-homogeneous deposits

Spatial and thickness non-uniformity



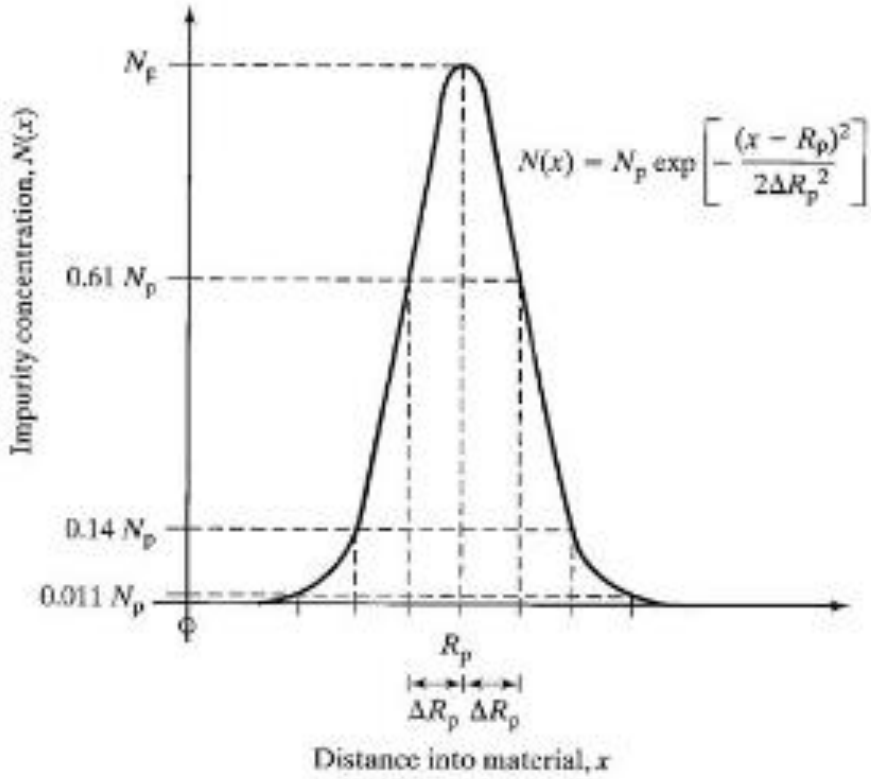
Eichfeld, *ACS Nano,* **9**, 2080 (2015)

Ion implantation

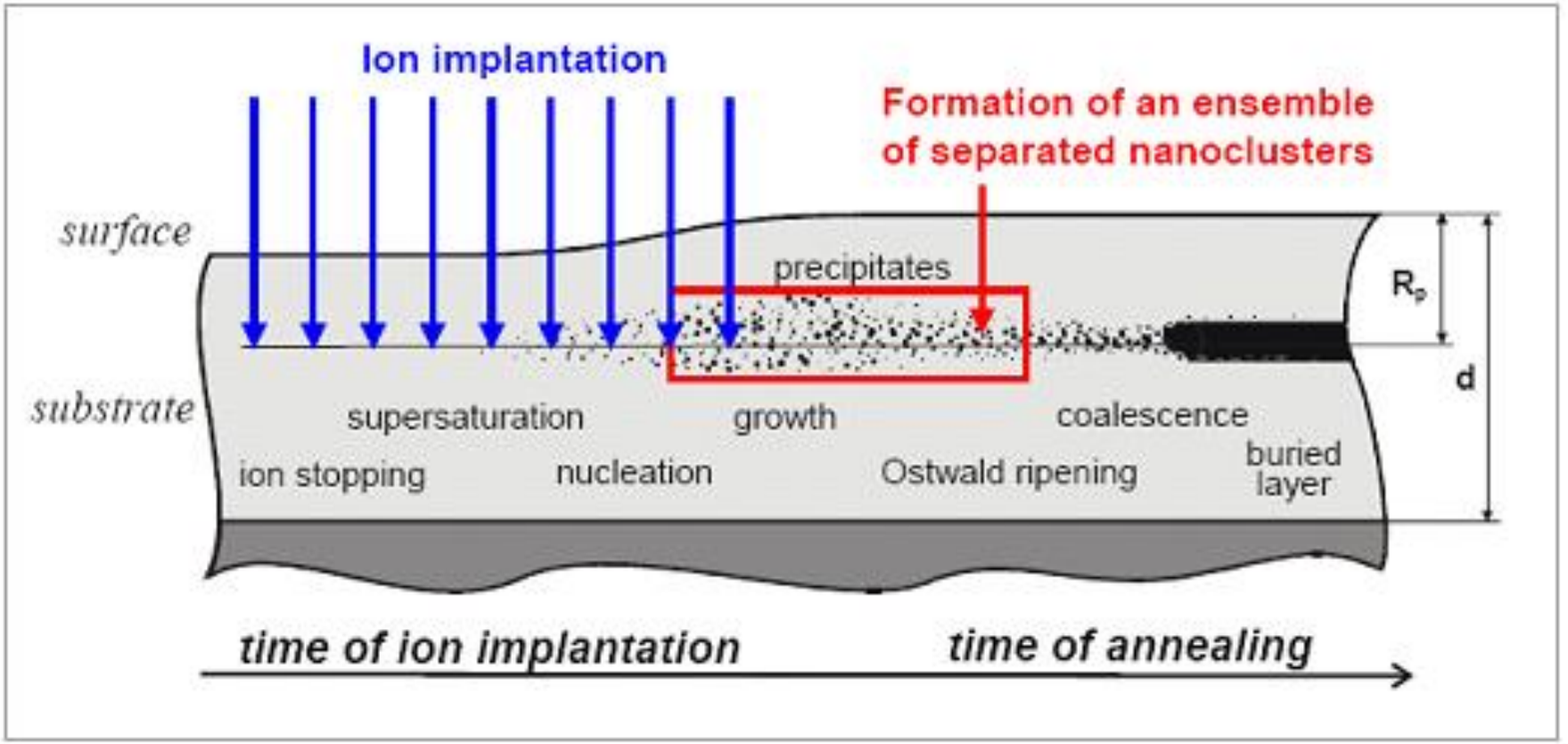


Advantages of Ion Implantation:

- Precise control of dose and depth profile
- Very fast (1 6" wafer can take as little as 6 seconds for a moderate dose)
- Wide selection of masking materials
  e.g. photoresist, oxide, poly-Si, metal
- Less sensitive to surface cleaning procedures
- Excellent lateral uniformity (< 1% variation across 12" wafer)

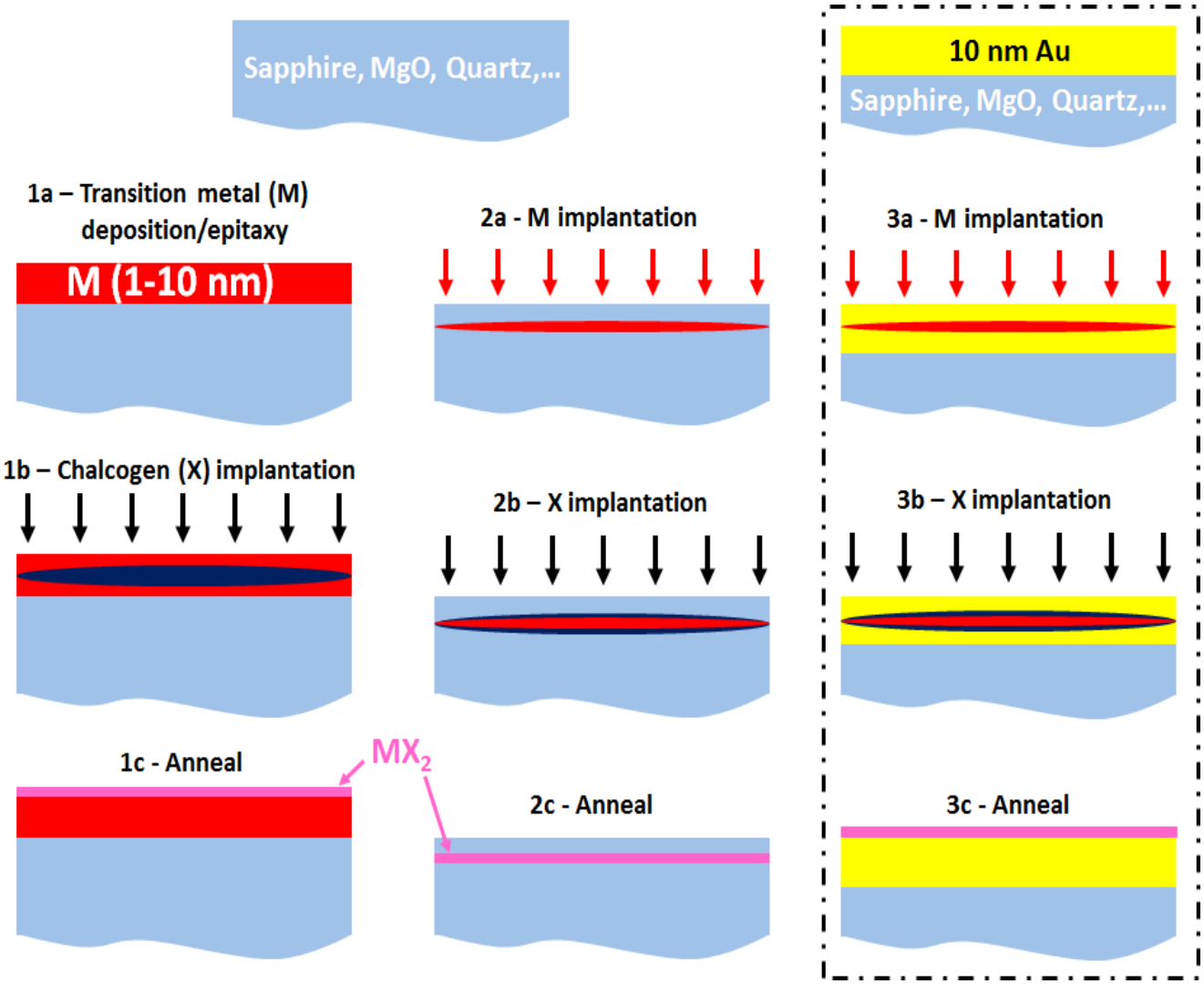


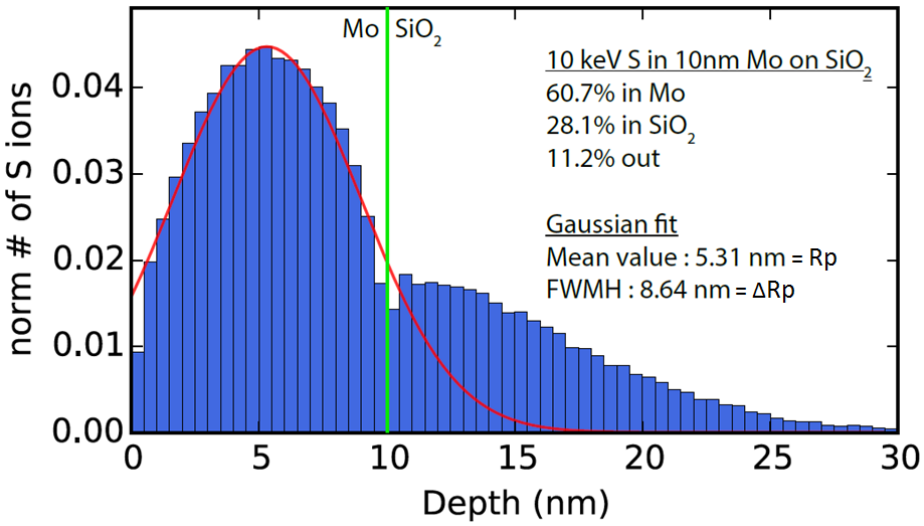
Simplified processes for ion implantation and annealing

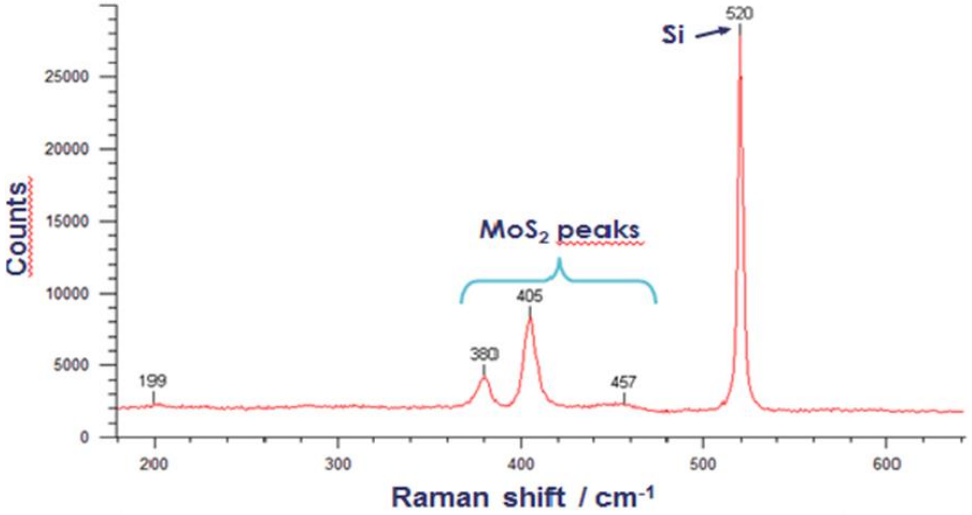


Adapted from Stepanov & Khaibullin, *Rev. Adv. Mater. Sci.*, **7,** 108 (2004)

SIMPLANT approaches

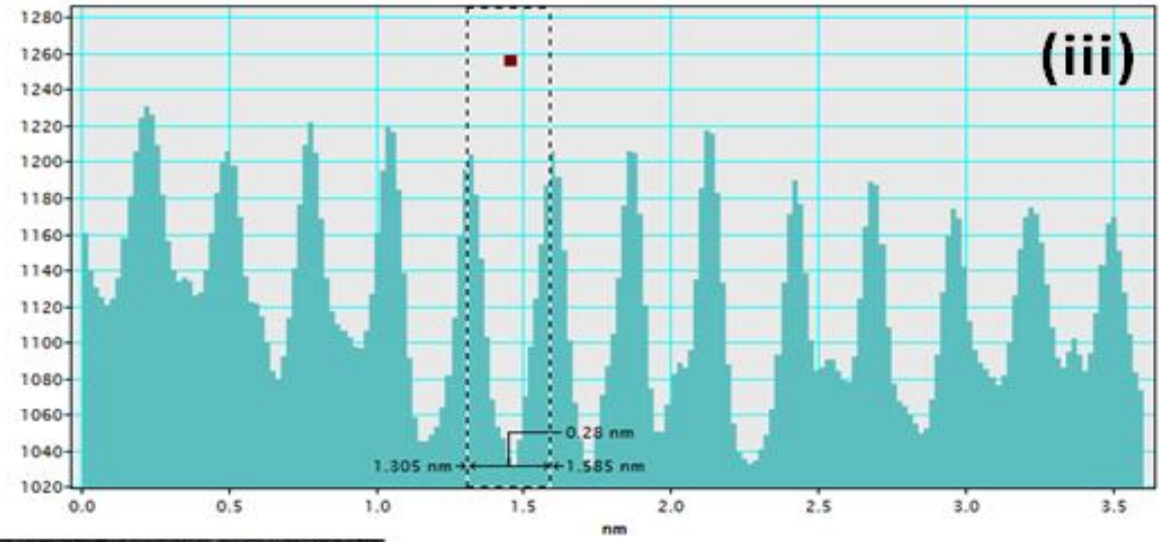


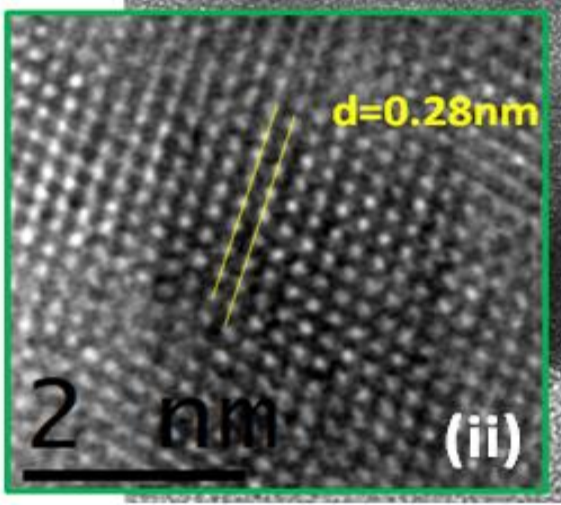




Preliminary Results

2.5 x 10^{15}/cm^2





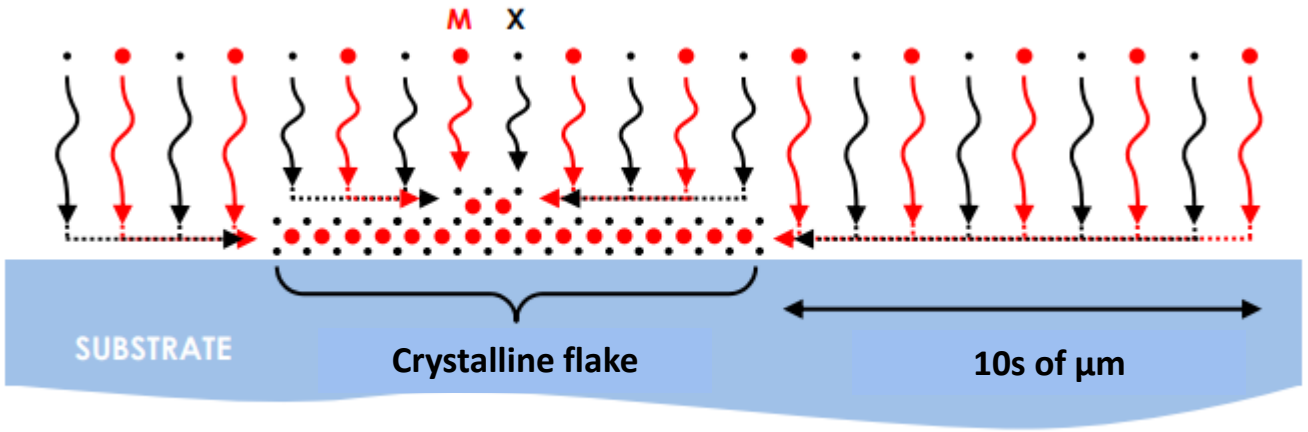
Unpublished

Simplified tasks' description

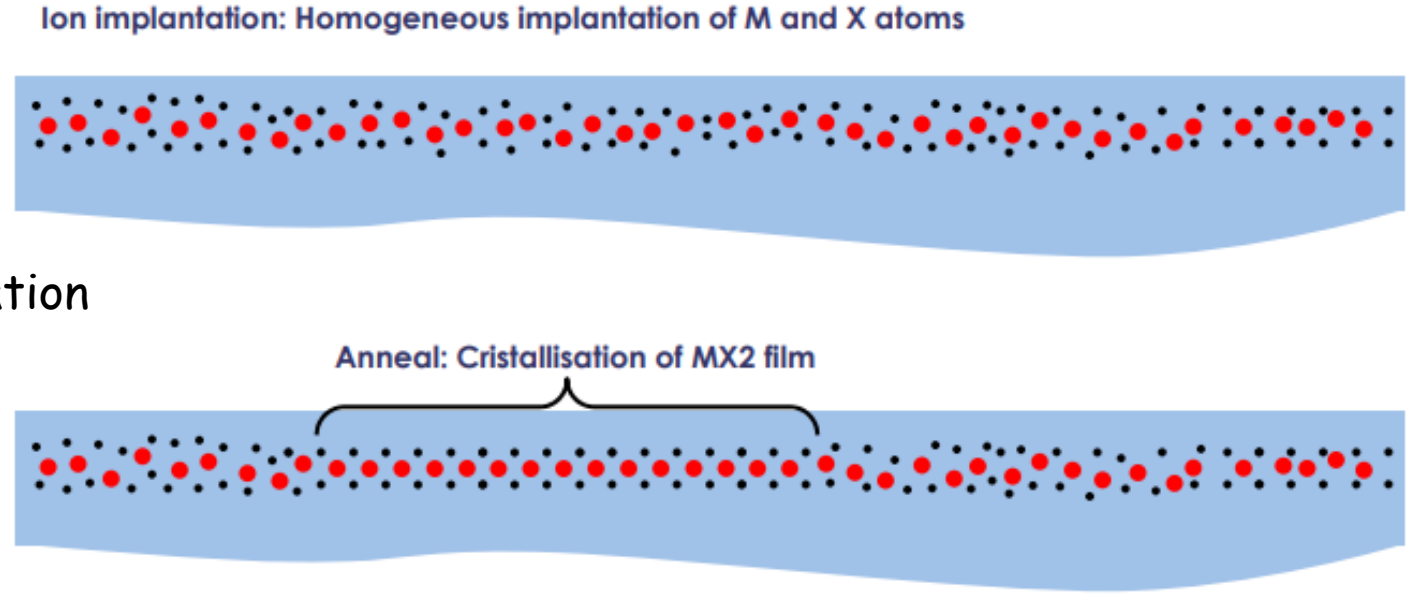
Tasks:

- **Metal epitaxy** (Mo, W on sapphire; Au on sapphire): INRP, TRT, LPICM
- **Ion Implantation**: INRP
- **Annealing**: INRP, LPICM, TRT, FHI
- **Characterizations**: FHI, TRT, LPICM, LSMP

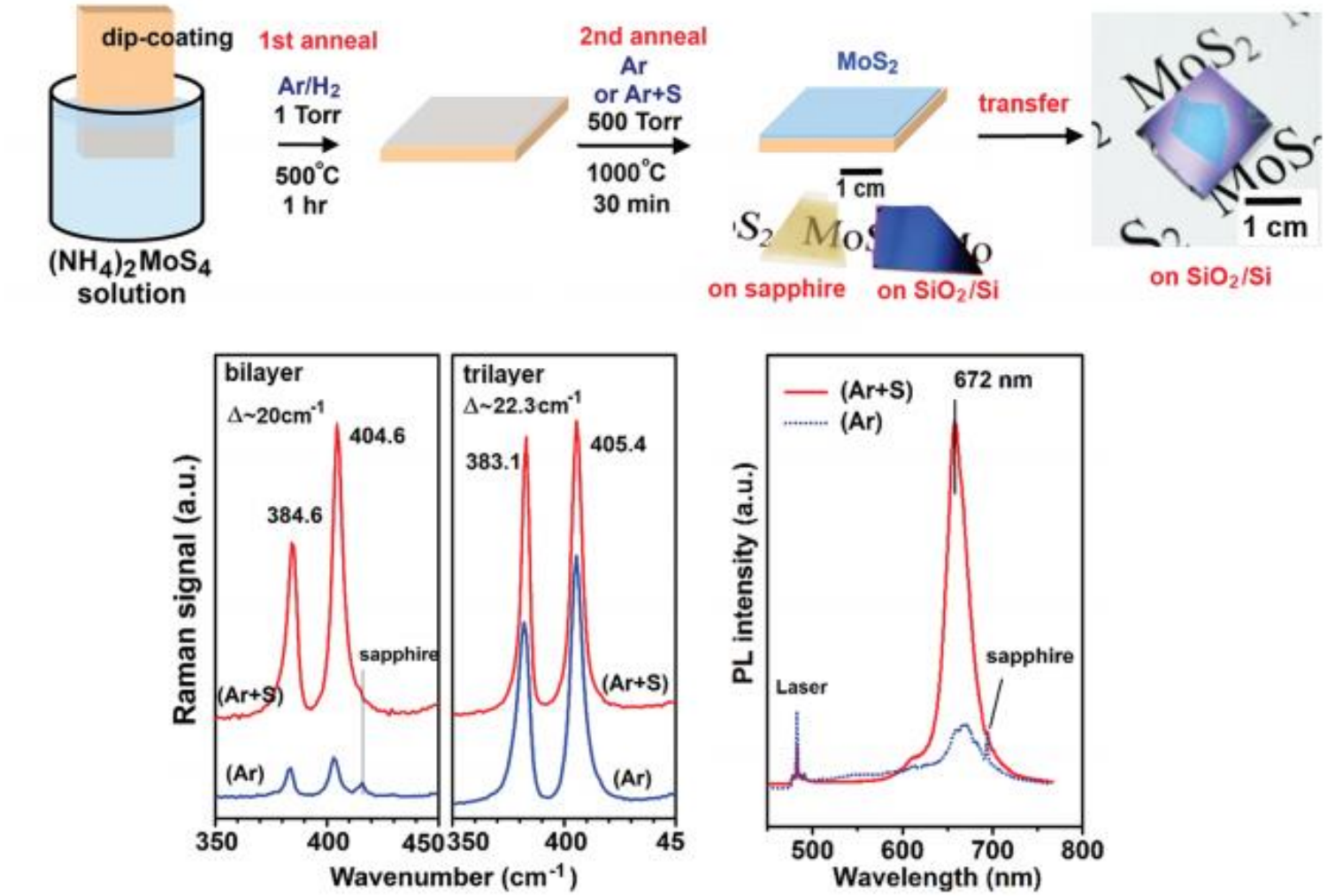
CVD growth



Ion implantation

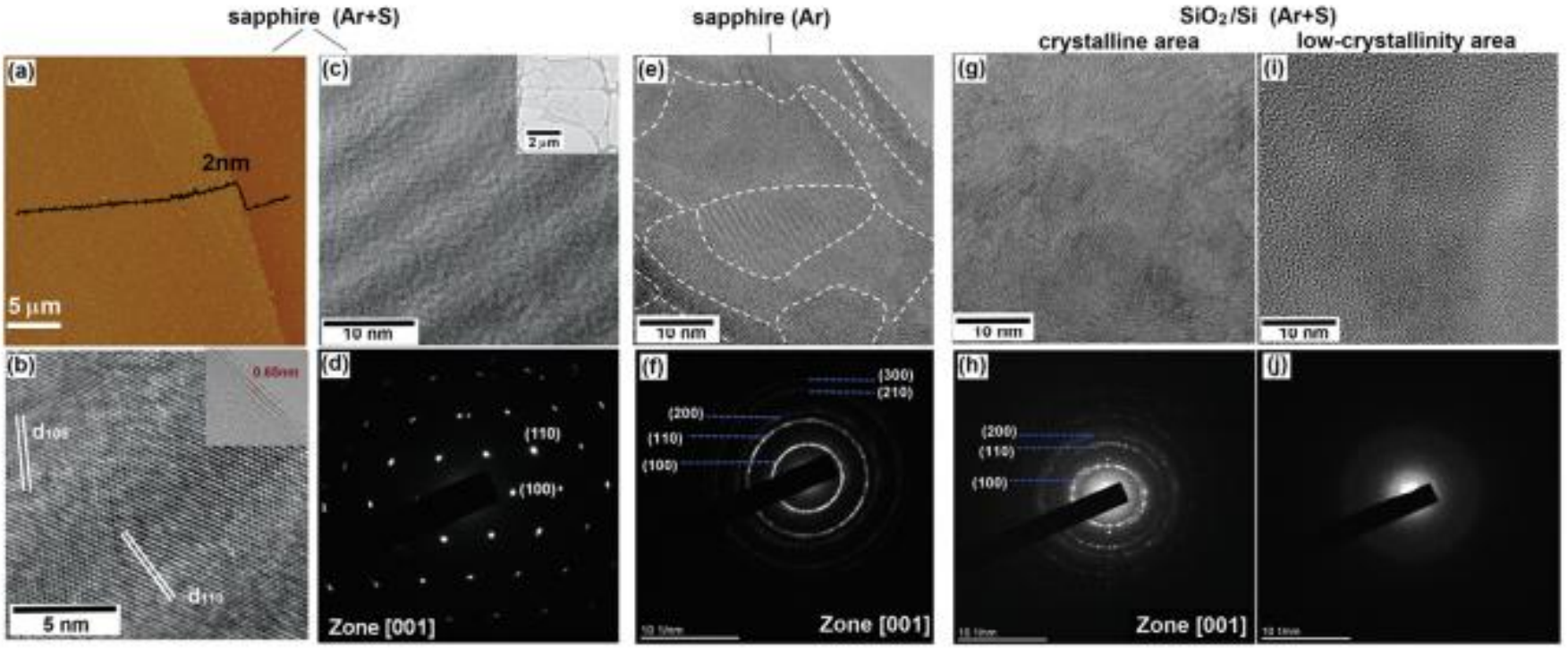


Direct decomposition of $(NH4)_2MoS_4$



Liu, *Nano Lett.*, **12**, 1538 (2012)

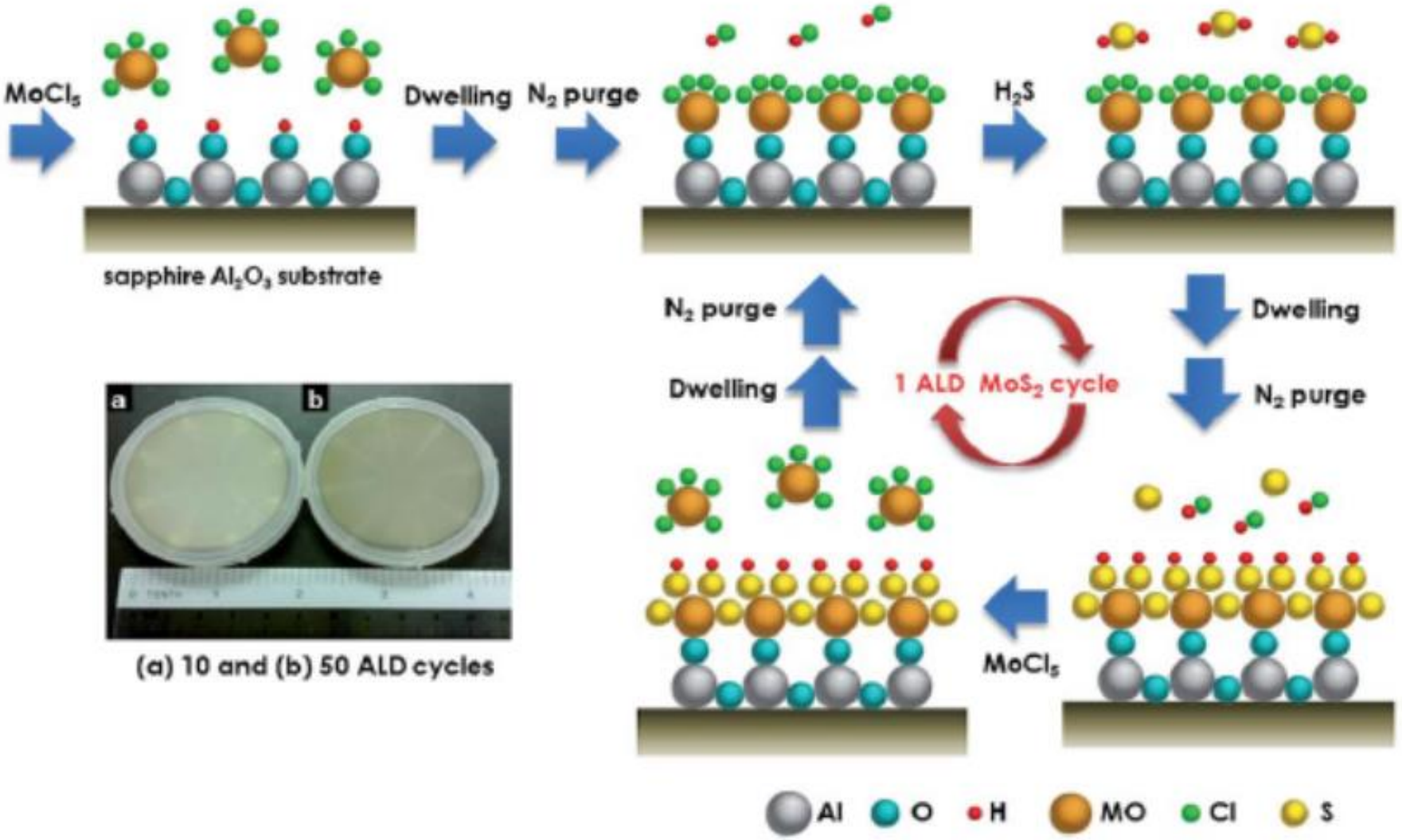
Direct decomposition of $(NH4)_2MoS_4$



Domain size for (Ar + S) anneal on sapphire: ~ 160 nm

Liu, *Nano Lett.*, **12**, 1538 (2012)

Atomic layer deposition



(a) 10 and (b) 50 ALD cycles

Tan, *Nanoscale*, **6**, 10584 (2014)

Bulk (3D) TMDC structures

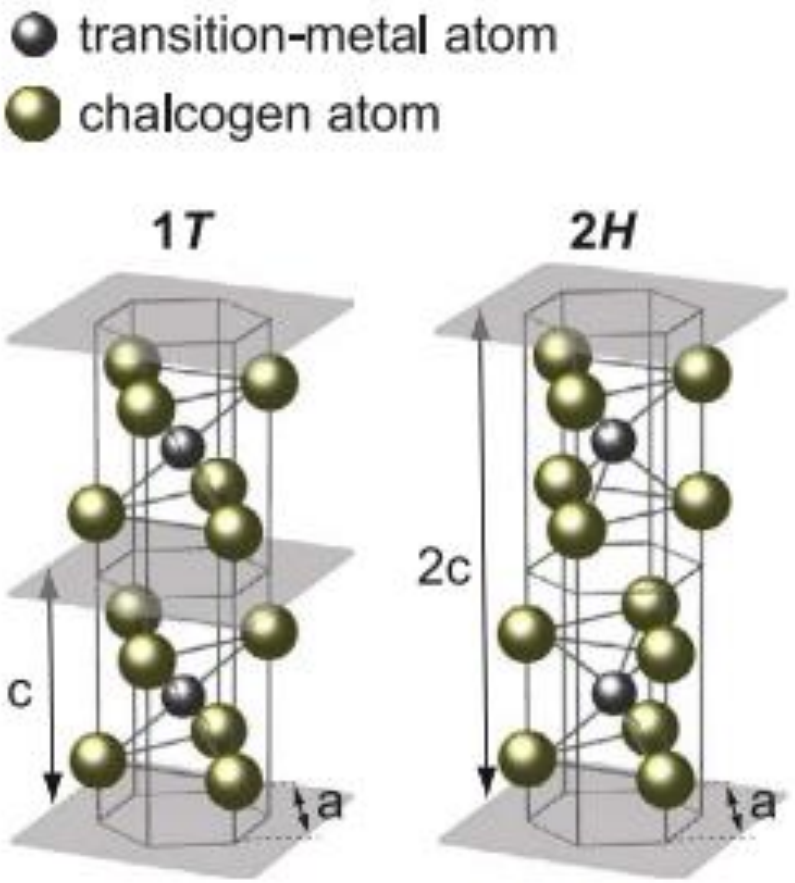


Figure 3. Schematic crystal structure of the 1T (left) and the 2H (right) polytype of layered transition-metal dichalcogenides. In the 1T structure, the transition-metal atoms are octahedrally coordinated by chalcogen atoms and the thickness of the repeat unit in the *c* direction is one sandwich. In the 2H structure, the coordination is trigonal prismatic and the unit cell is two sandwiches thick.

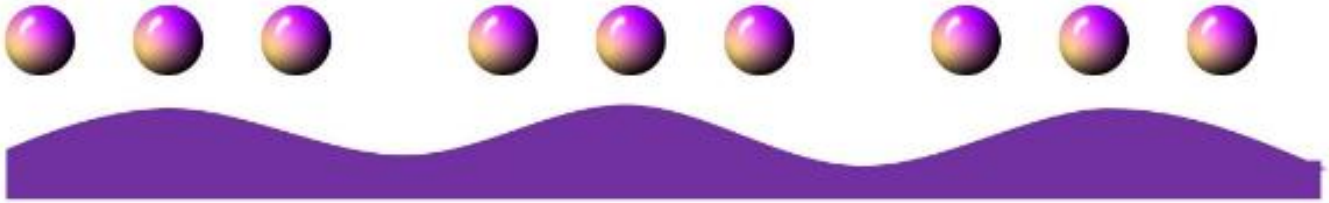
Ions uniformly spaced

$T > T_C$

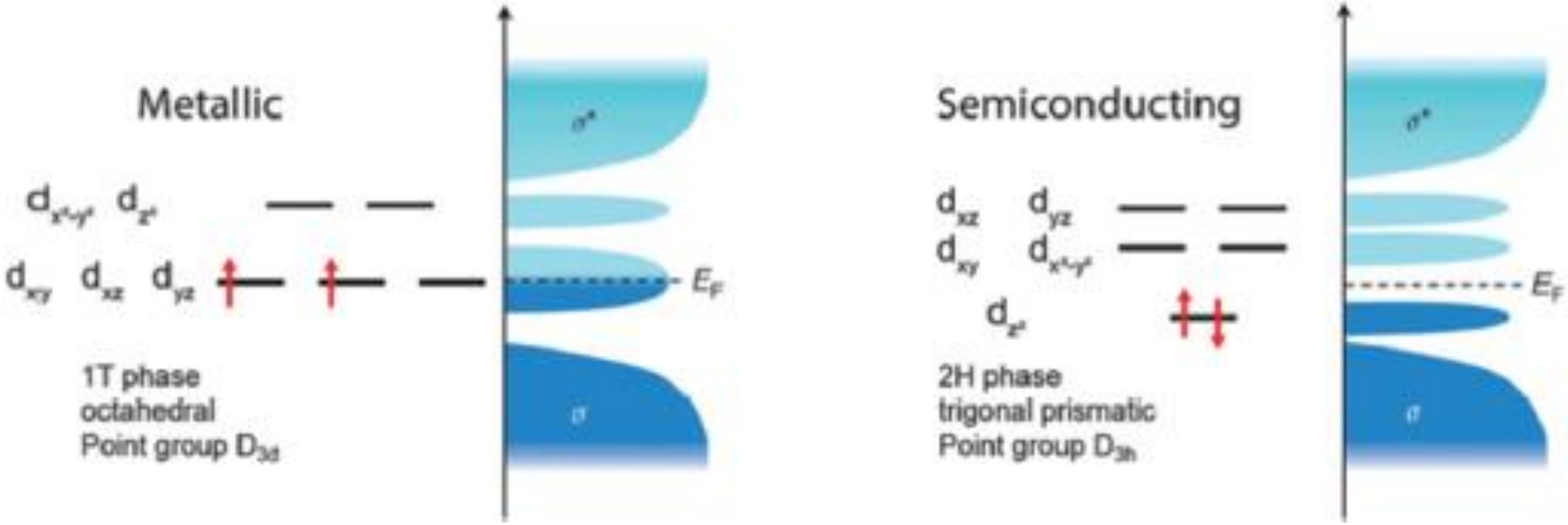
Uniform electron density

Static periodic lattice distortion

$T < T_C$



Modulated electron density (charge density wave)


Metallic
$d_{x^2-y^2}$ d_{z^2}
d_{xy} d_{xz} d_{yz}
E_F
1T phase
octahedral
Point group D_{3d}
σ^*
σ
Semiconducting
d_{xz} d_{yz}
d_{xy} $d_{x^2-y^2}$
d_{z^2}
E_F
2H phase
trigonal prismatic
Point group D_{3h}
σ^*
σ