

Epitaxial growth of single-crystal hexagonal boron nitride monolayer on copper

Yifan Yuan

Group meeting

04/19/2021

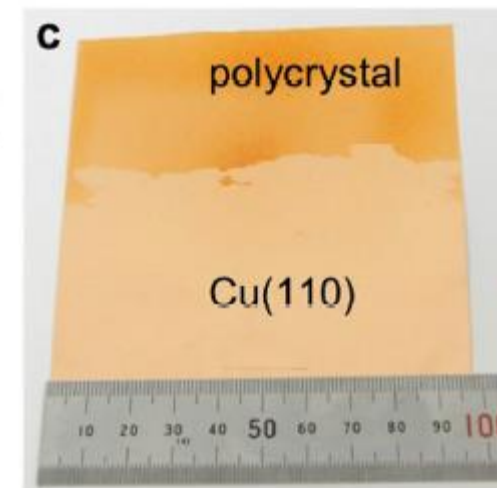
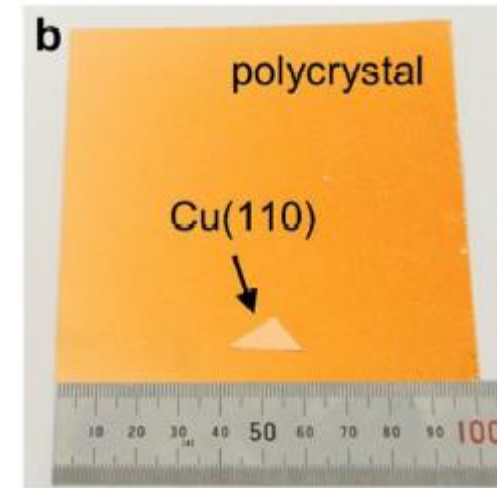
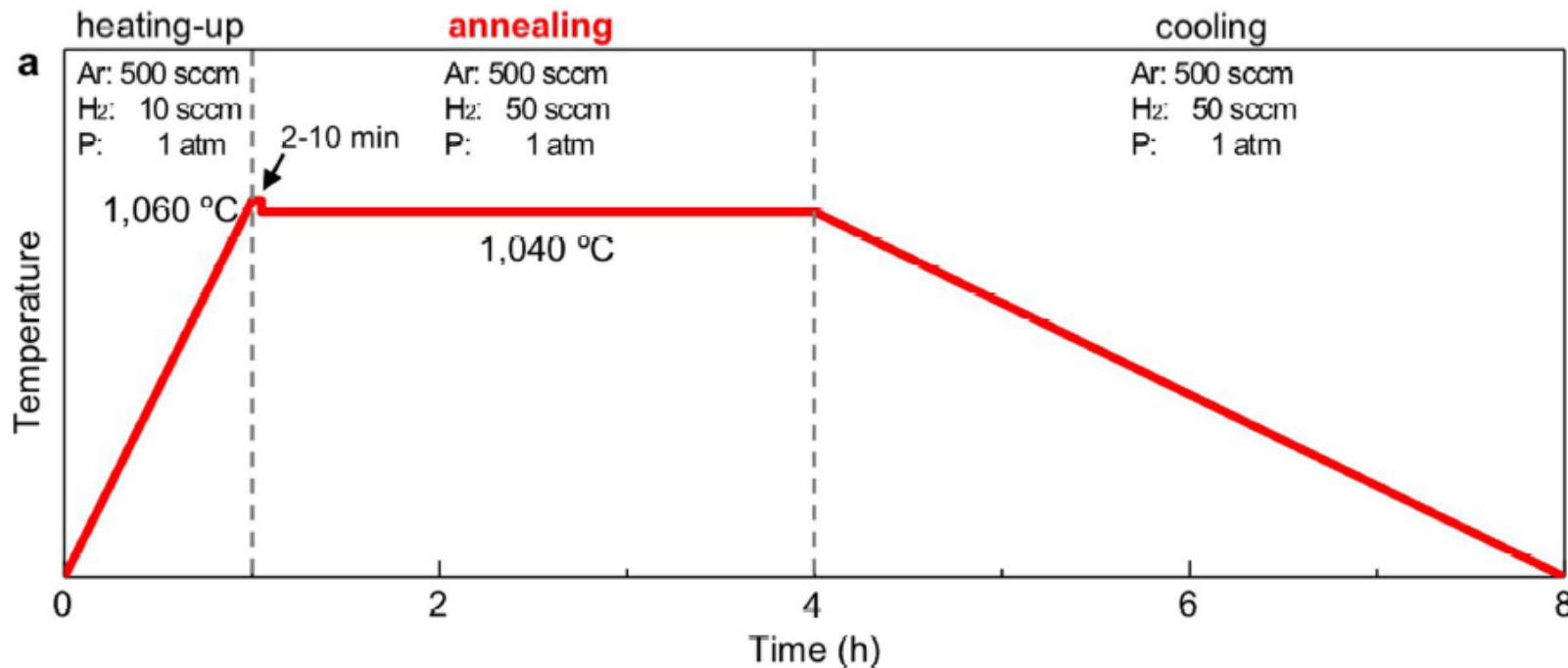
Wang, L., Xu, X., Zhang, L. *et al.* Epitaxial growth of a 100-square-centimetre single-crystal hexagonal boron nitride monolayer on copper. *Nature* **570**, 91–95 (2019).

<https://doi.org/10.1038/s41586-019-1226-z>

Annealing of a $10 \times 10 \text{ cm}^2$ single-crystal Cu (110) foil

1. Anneal polycrystalline Cu foil at $1060 \text{ }^\circ\text{C}$ for 2–10 min under a mixed-gas flow (Ar, H_2) to melt surface
2. Put a single-crystal Cu (110) foil on the surface as an artificial seed,
3. Anneal Cu foils at $1040 \text{ }^\circ\text{C}$ for 3 h.

Melting point of Cu: $1085 \text{ }^\circ\text{C}$



Growth of 10 × 10 cm² single-crystal 2D hBN films

Precursor: Ammonia borane (BH₃NH₃)

CVD

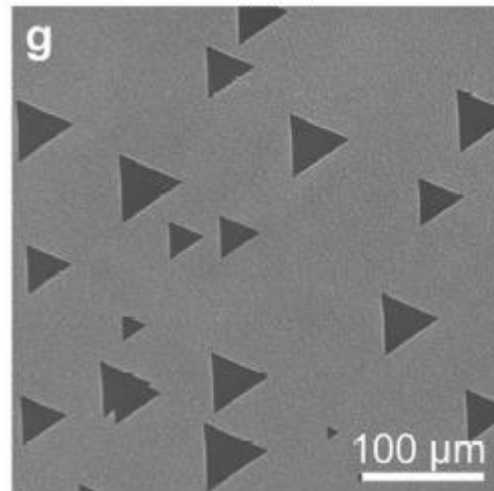
Substrate temperature 1,035 °C

Source temperature: 65 °C

Pressure: 200 Pa with Ar (5 sccm) and H₂ (45 sccm)

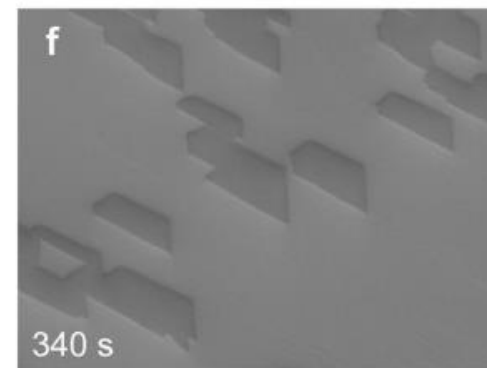
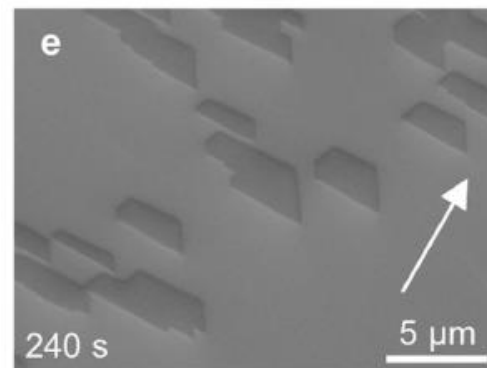
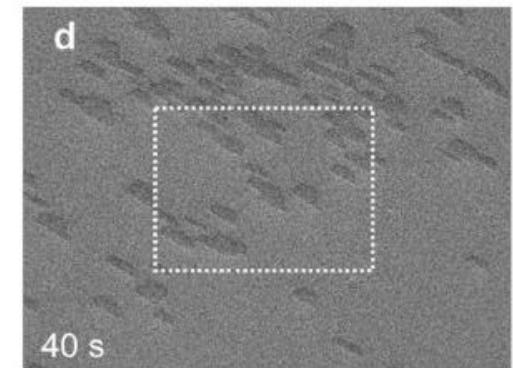
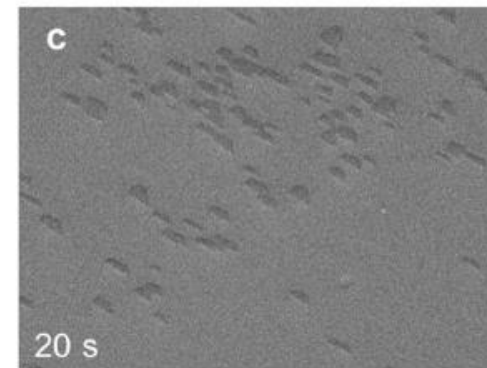
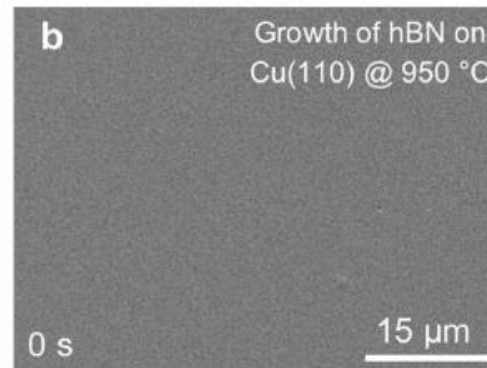
Growth time: 1 h for individual hBN domains; 3 h for a continuous hBN film

SEM image



Epitaxial hBN on Cu (110)

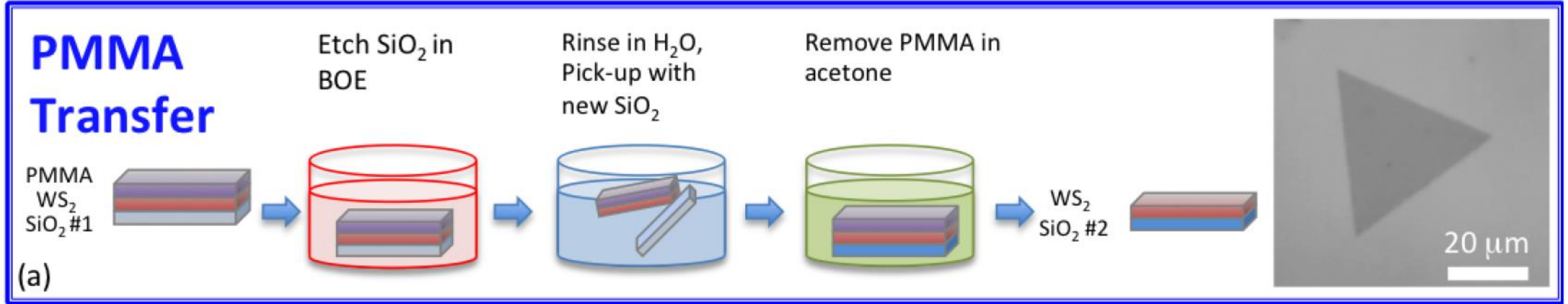
Unidirectional aligned domains



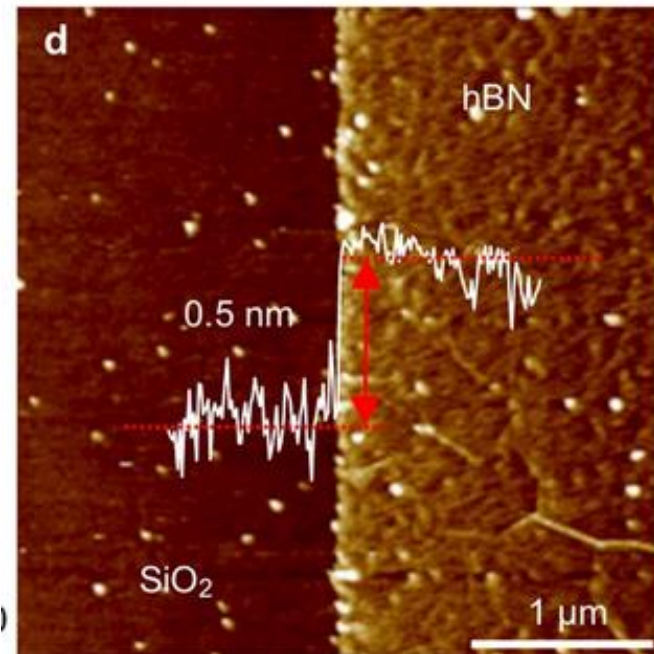
In situ observation of growth

Transfer of hBN films

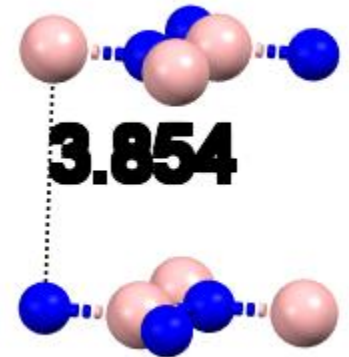
the polymethyl-methacrylate-based transfer technique.



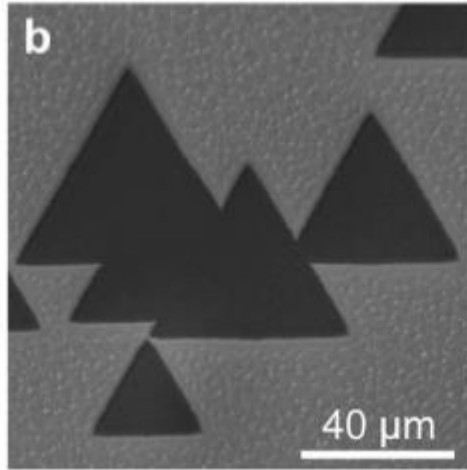
BOE: buffered oxide etchant



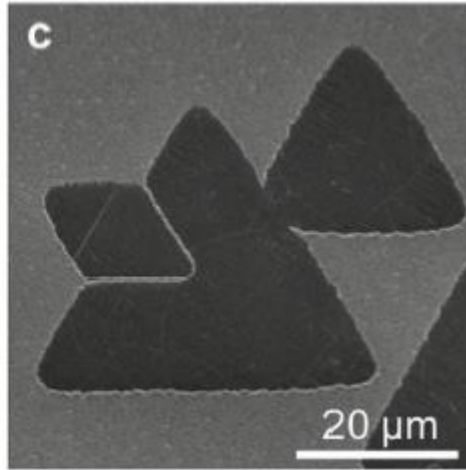
Monolayer thickness



SEM after H₂ etching

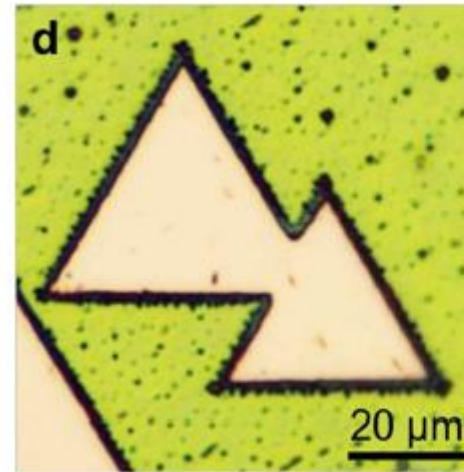


Cu (110) / hBN

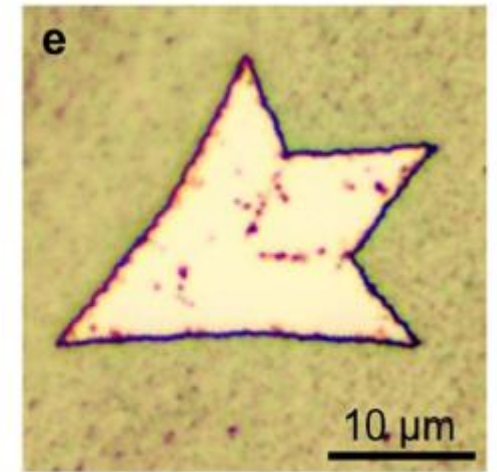


Cu (111) / hBN

OM after UV oxidation



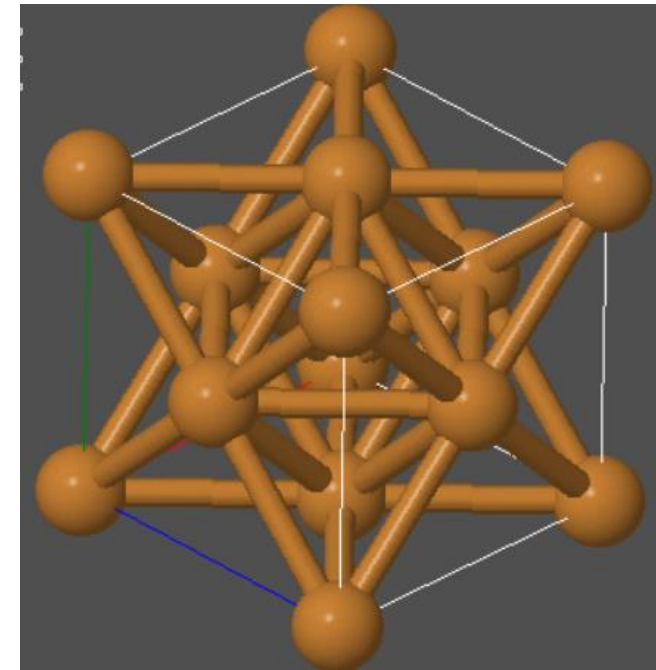
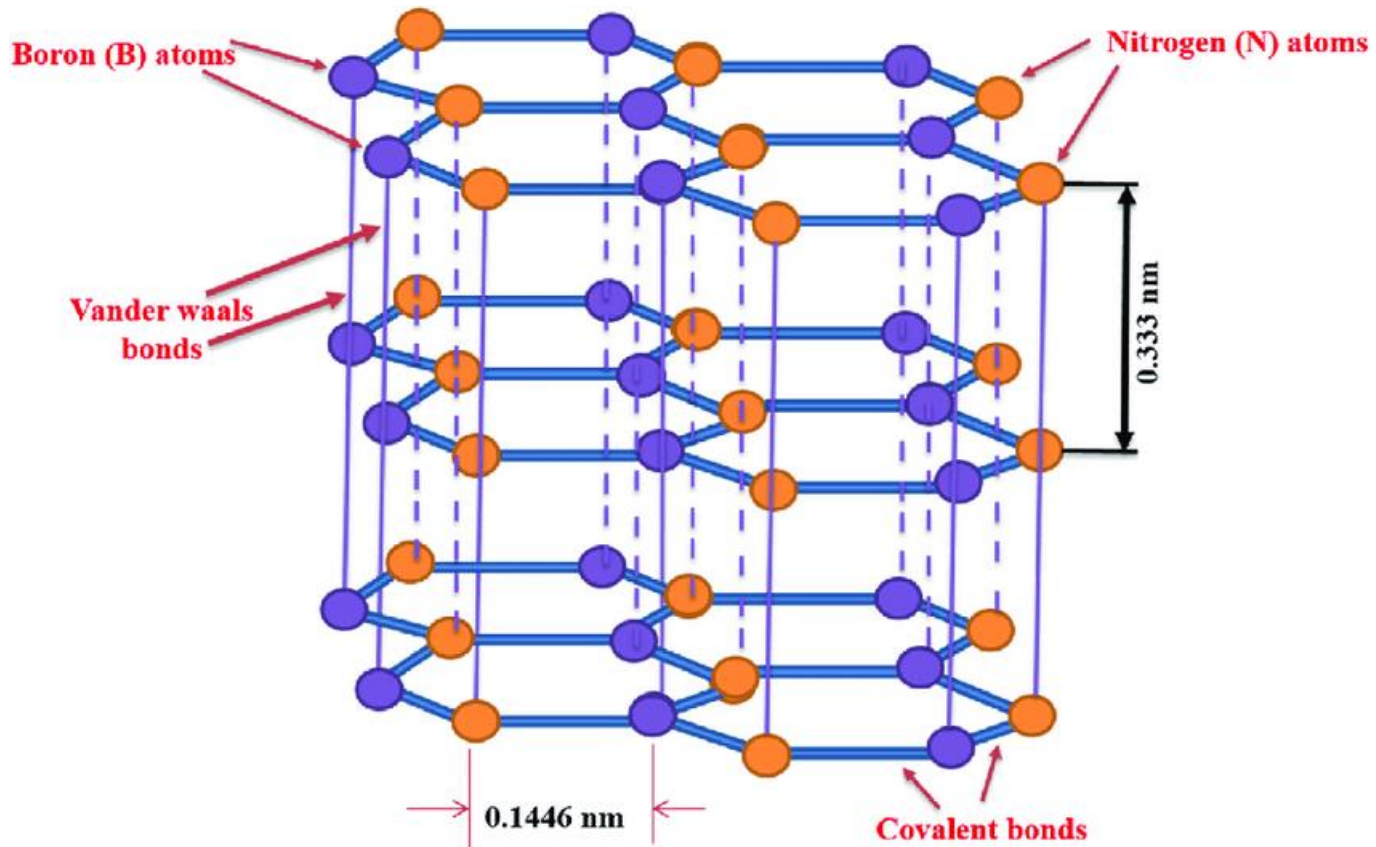
Cu (110) / hBN
No boundary line



Cu (111) / hBN
a 60° twist angle

Why can hBN be epitaxial on Cu(110), not on Cu (11)?

hBN structure (C_{3v} symmetry) is not compatible with the C_{6v} symmetry of the top-layer atoms of the Cu (111) surface

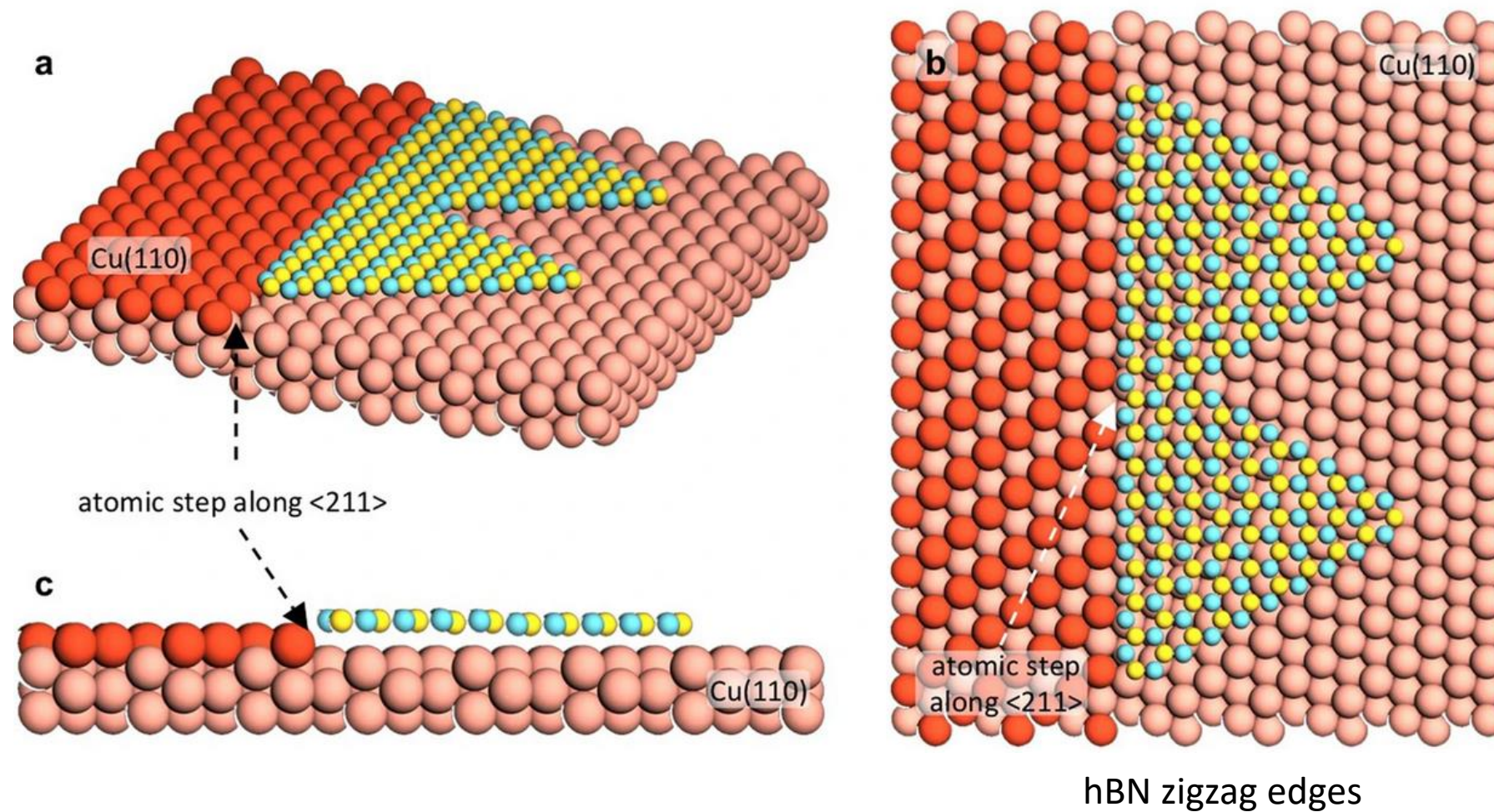


Cu, FCC

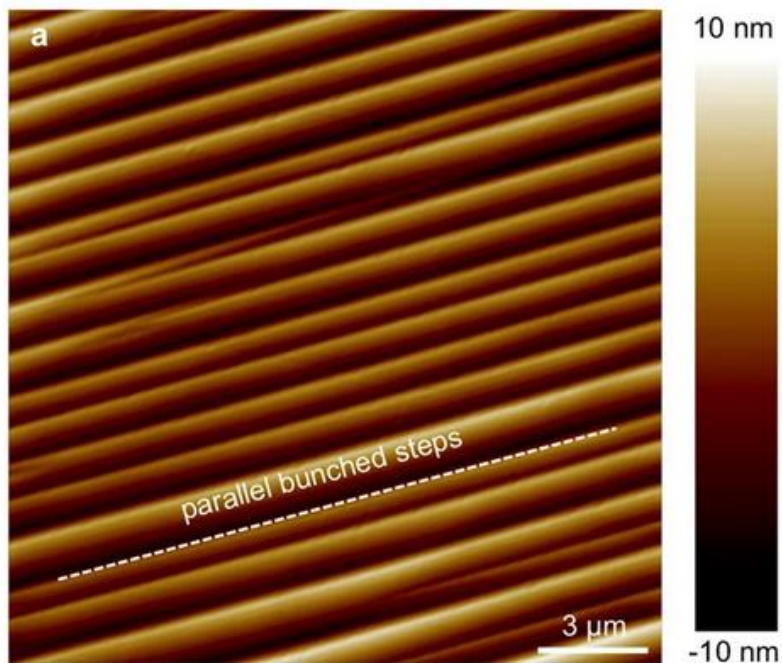
hBN structure (C_{3v} symmetry) is compatible with C_{3v} , C_3 , σ_v or C_1 symmetry.

The edge-coupling-guided growth mechanism

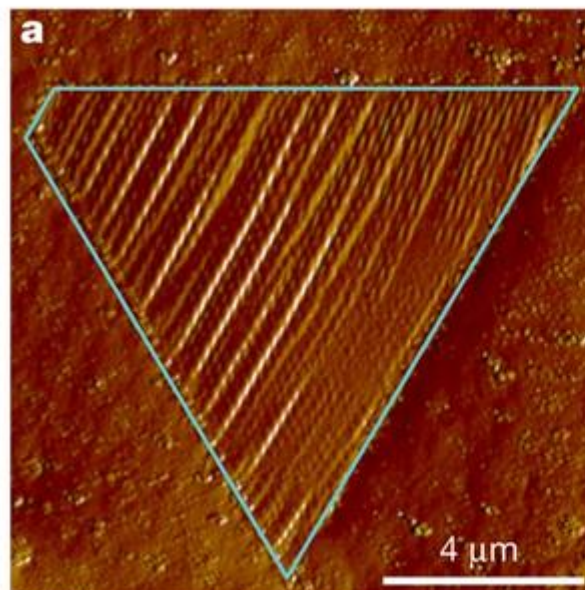
Cu (110) vicinal surface, on which the presence of metal steps along the $\langle 211 \rangle$ direction led to a C_1 symmetry.



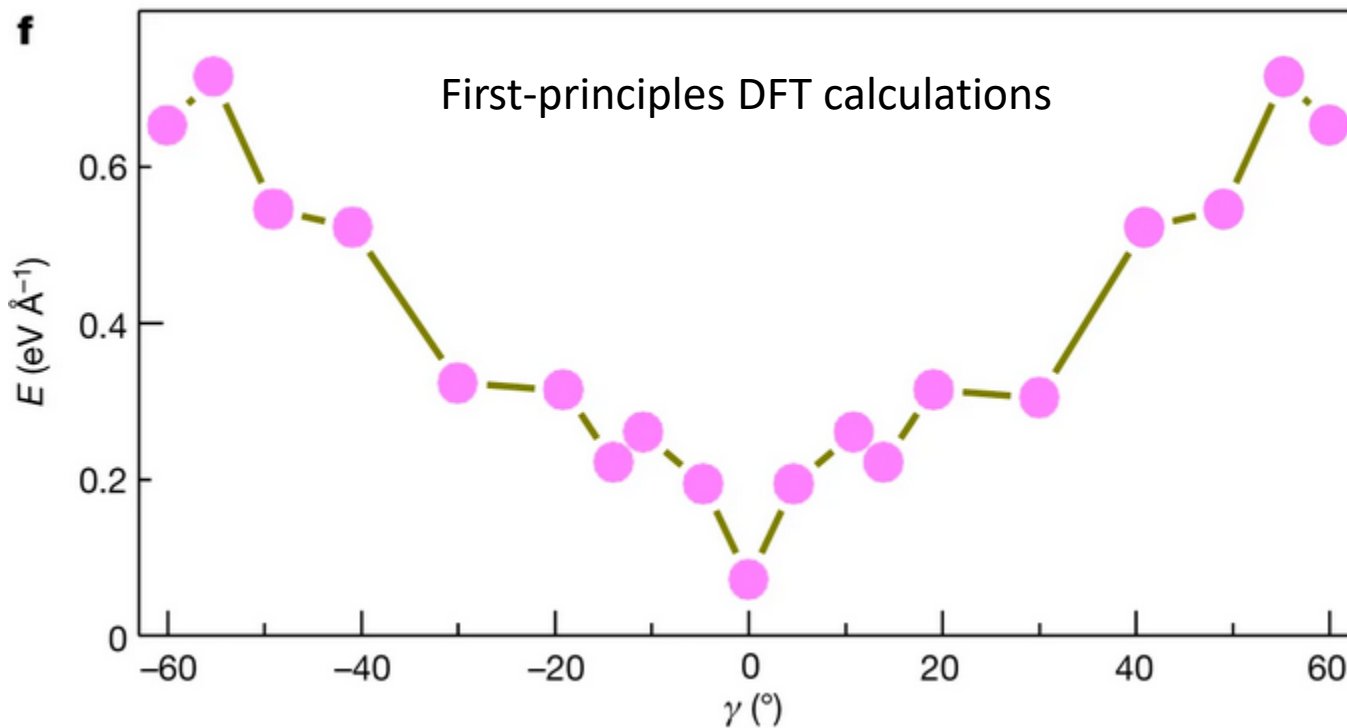
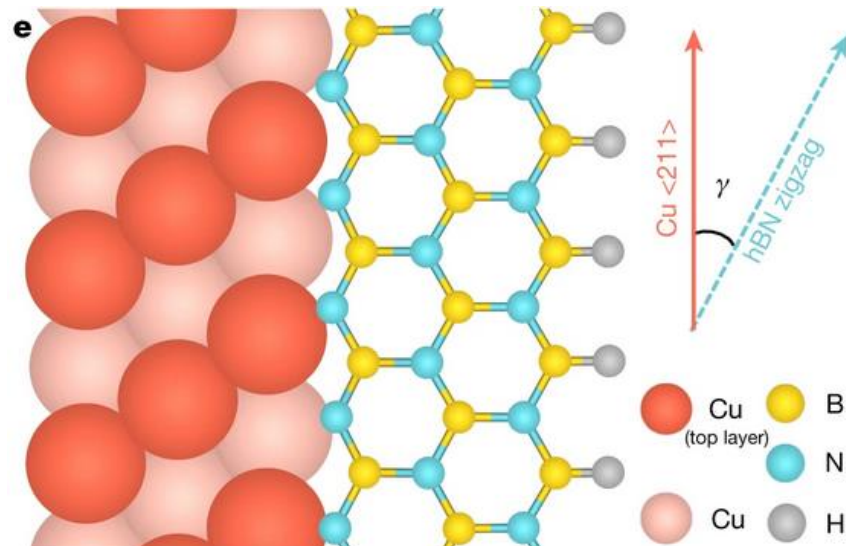
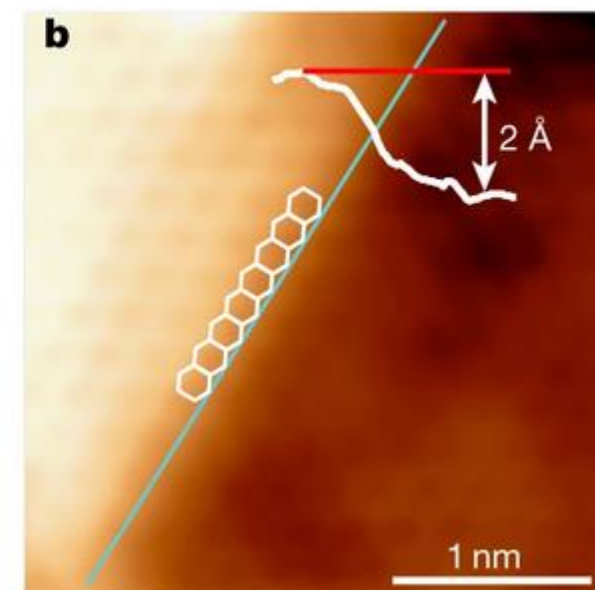
AFM images of parallel bunched steps on a bare as-annealed Cu surface

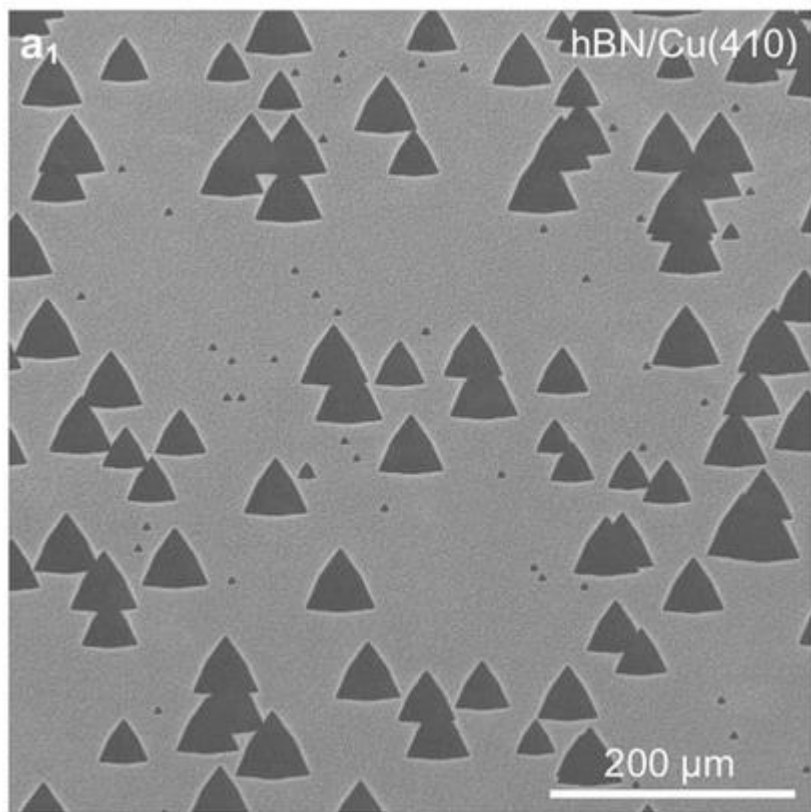


AFM phase image

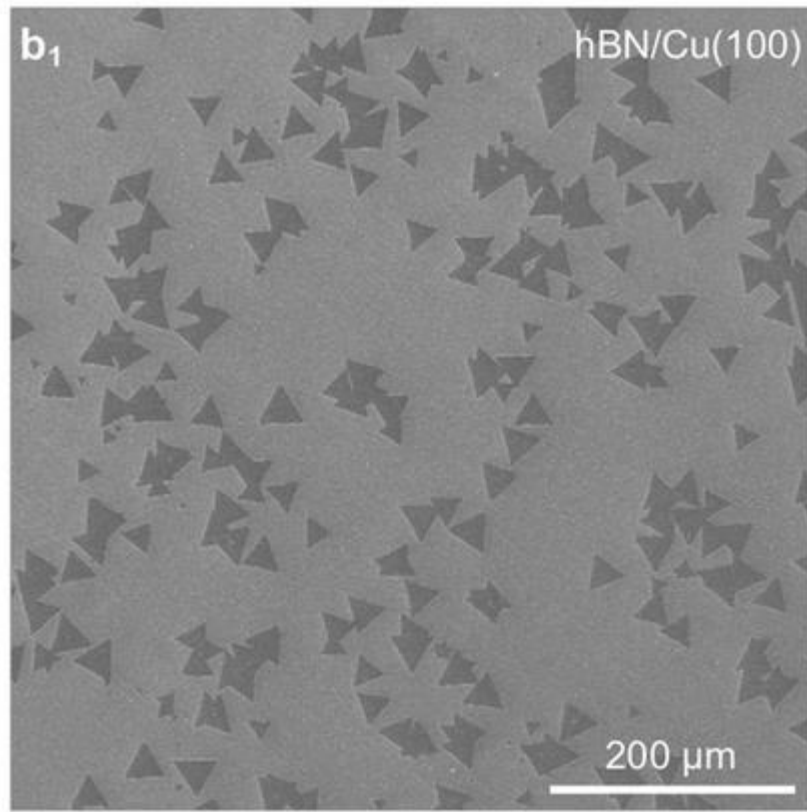


STM image

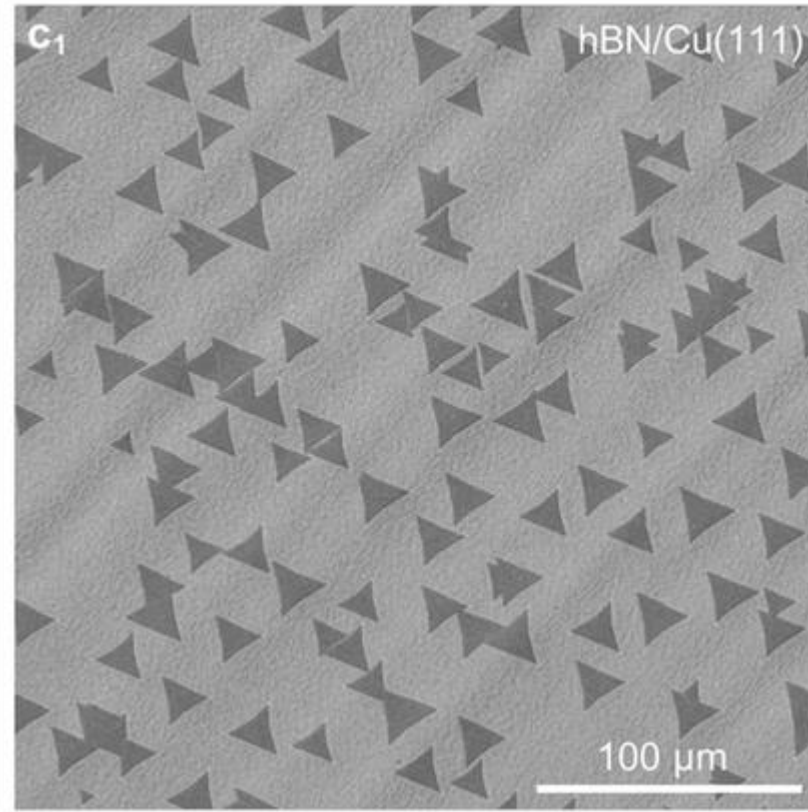




unidirectionally aligned growth



randomly aligned hBN domains



anti-parallel domains

Ferroelectricity of HCl family

Yifan Yuan

Group meeting

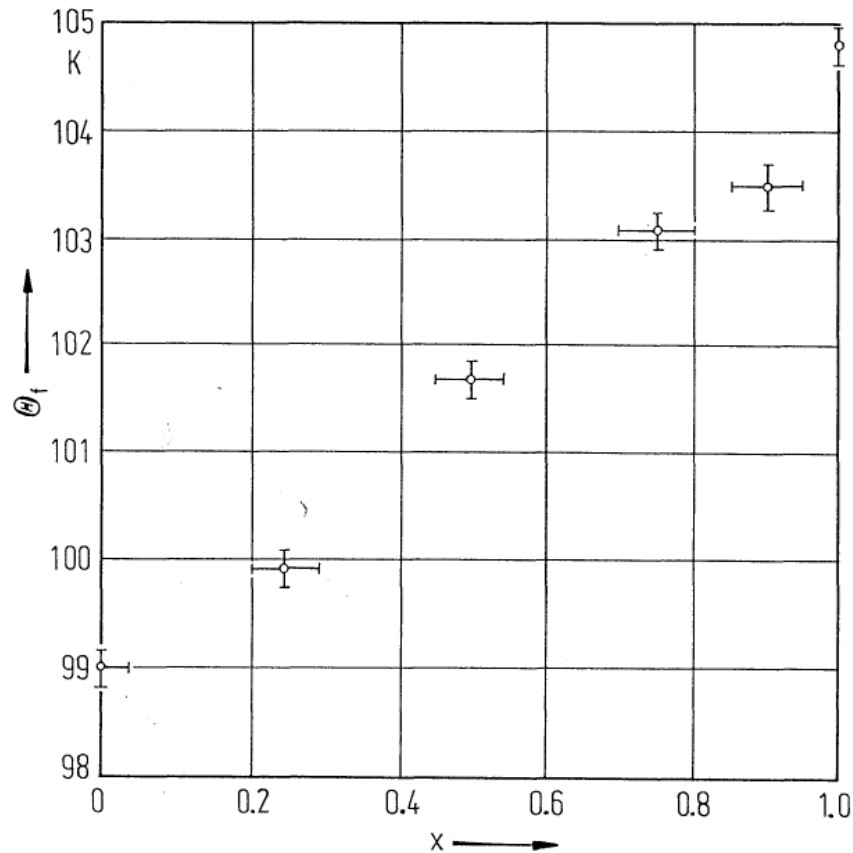
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HCl crystals

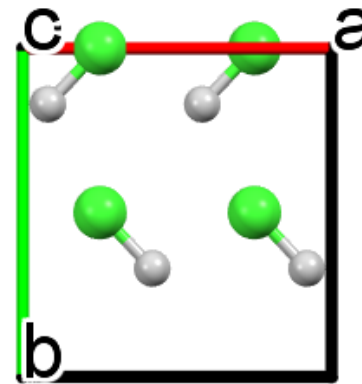
Ferroelectricity in HCl was discovered by Hoshino et al. in 1967.

Melting point: 158.91 K (DCl: 158.44 K) Deuterium

Curie temperature: 98.36 ° [D: 105.03 °] K



Ferroelectric orthorhombic phase, $Bb2_1m$



Order-disorder ferroelectric

Paraelectric cubic phase, $Fm3m$

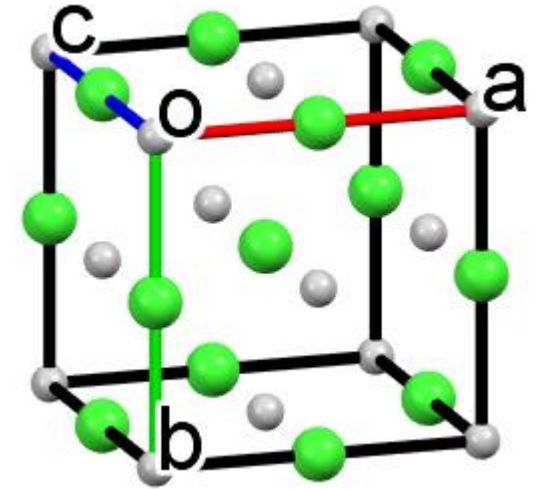


Fig. 27A-1-001. $H_{1-x}D_xCl$. Θ_f vs. x [83Cro].

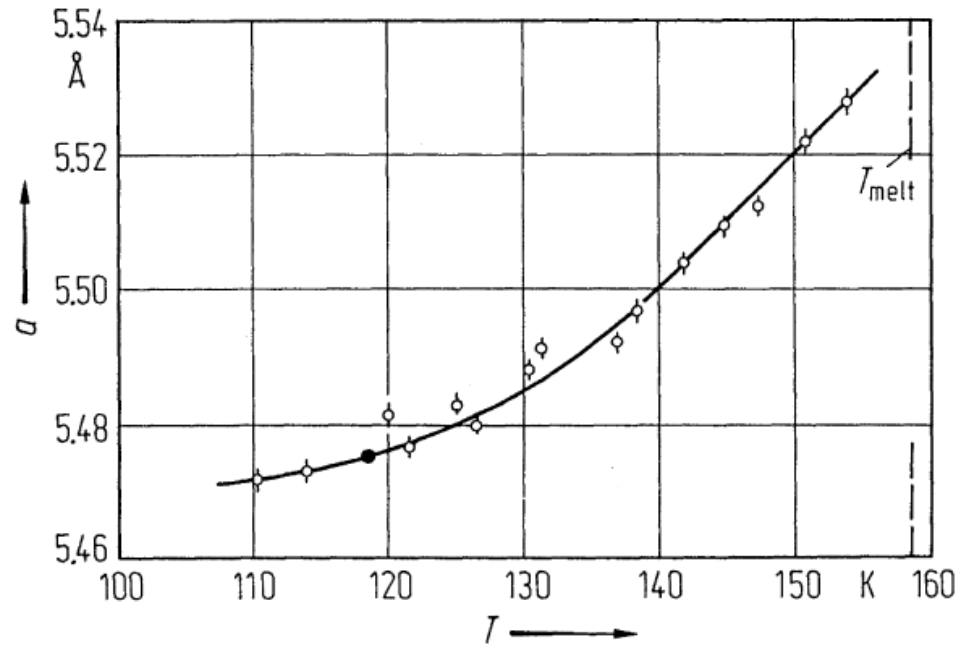


Fig. 27A-1-004. DCl. a vs. T [73Nii]. Data are normalized

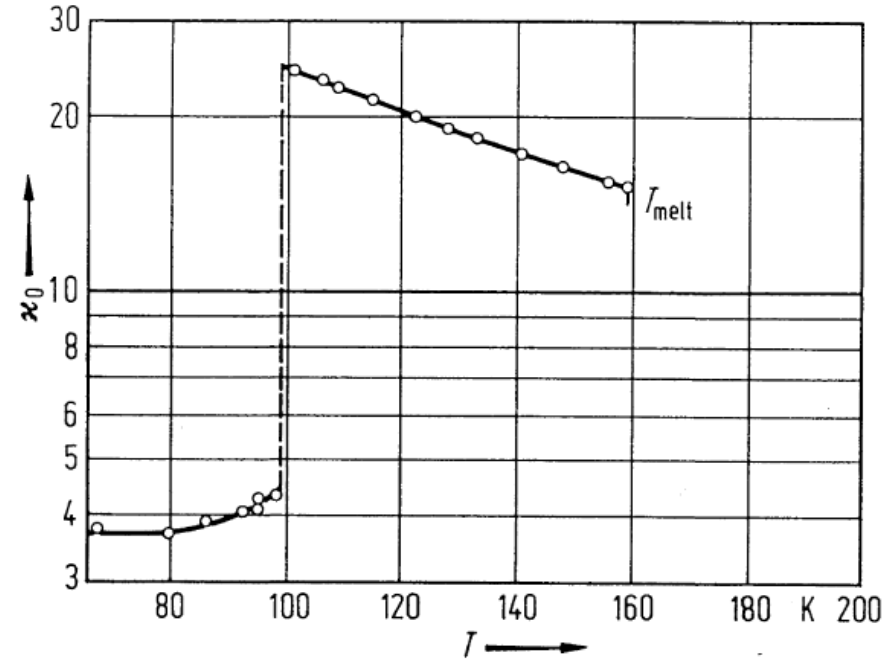


Fig. 27A-1-005. HCl (polycrystal). κ_0 vs. T [54Swe]. κ_0 : static dielectric constant.

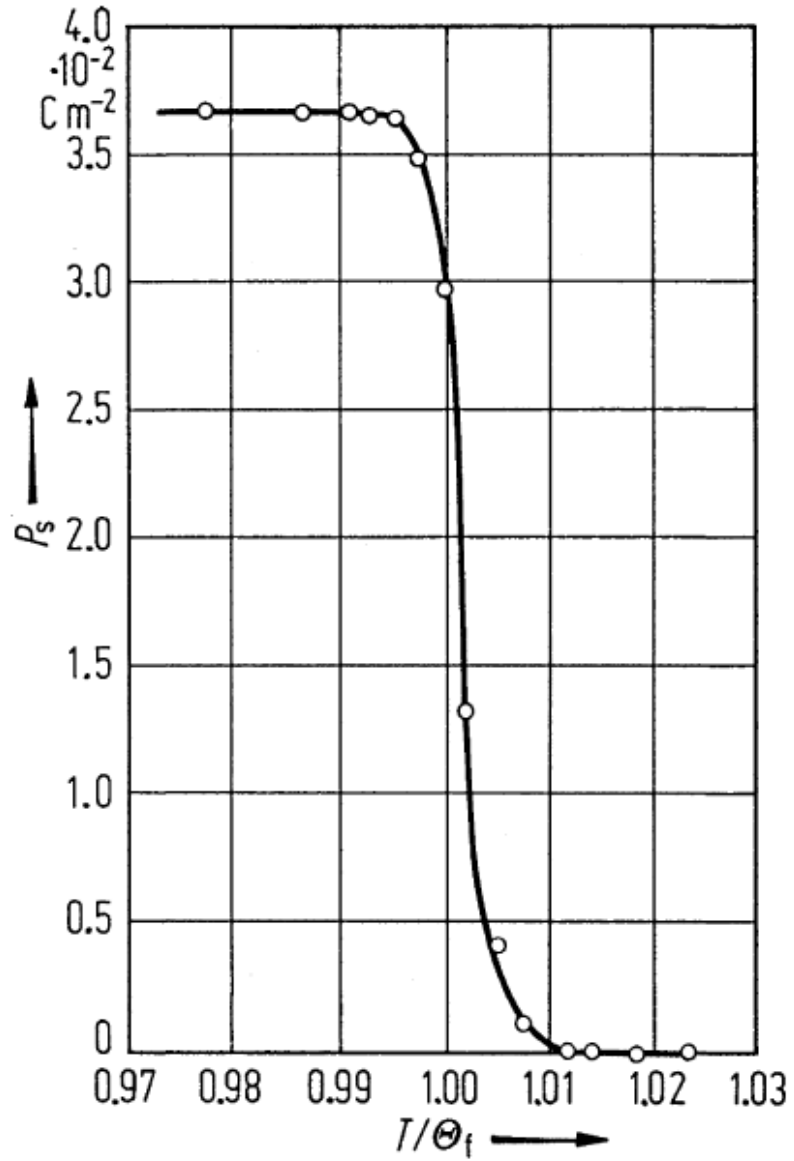
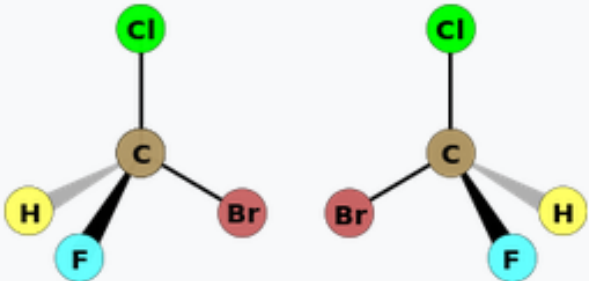
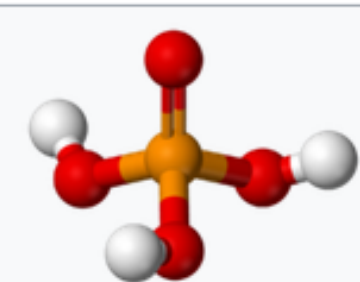



Fig. 27A-1-007. HCl. P_s vs. T/Θ_f [69Kol]

Point group	Symmetry operations ^[15]	Simple description of typical geometry	Example 1
C_1	E	no symmetry, chiral	 <p data-bbox="1541 464 2331 564">bromochlorofluoromethane (both enantiomers shown)</p>
C_3	E C_3	propeller, chiral	 <p data-bbox="1796 906 2076 949">phosphoric acid</p>
C_{3v}	E $2C_3$ $3\sigma_v$	trigonal pyramidal	 <p data-bbox="1719 1249 2127 1292">non-inverting ammonia</p>