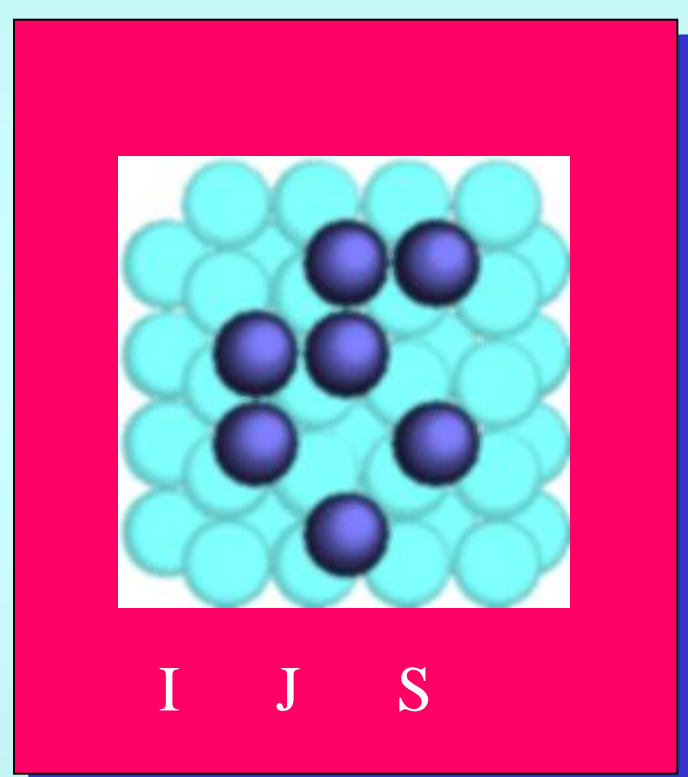


The surface structures of some transition-metal dichalcogenides



Albert Prodan and Horst Böhm

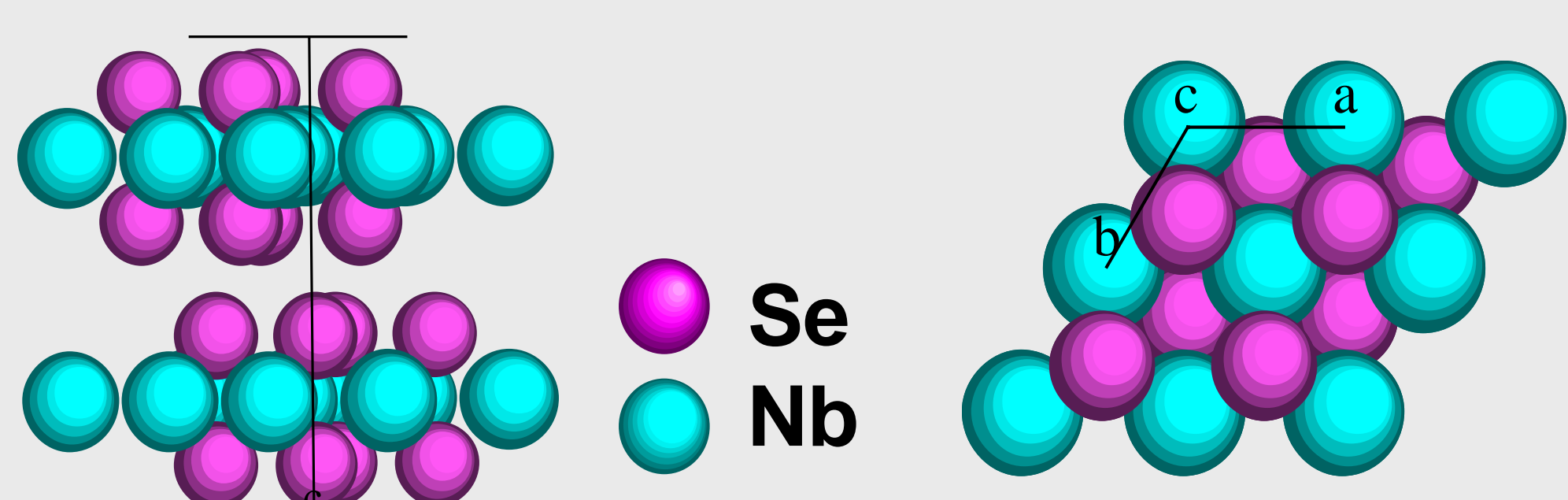
Institute Jožef Stefan, Ljubljana, Jamova 39, SI-1000 Slovenia

Institut für Geowissenschaften, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany.



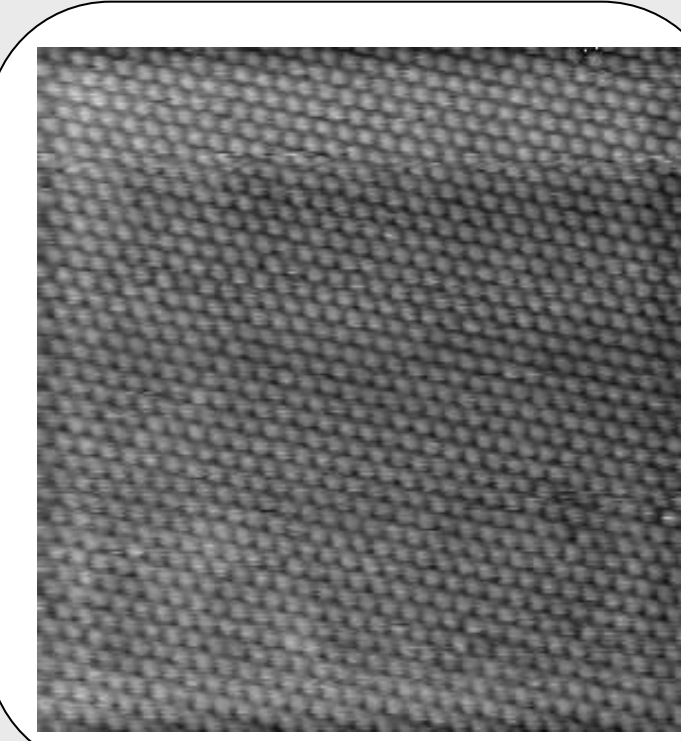
Acknowledgment: The work is financially supported by the Materialwissenschaftliches Forschungszentrum der Johannes-Gutenberg-Universität Mainz and by the "DLR Internationales Büro" Bonn

The basic structure of NbSe₂

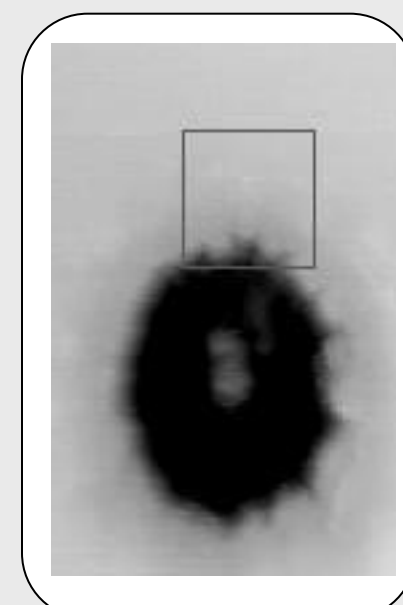


SG = P6₃/mmc, Z=2, a₀=3.4446 Å,
c₀=12.5444 Å
2H_a-NbS₂ - type

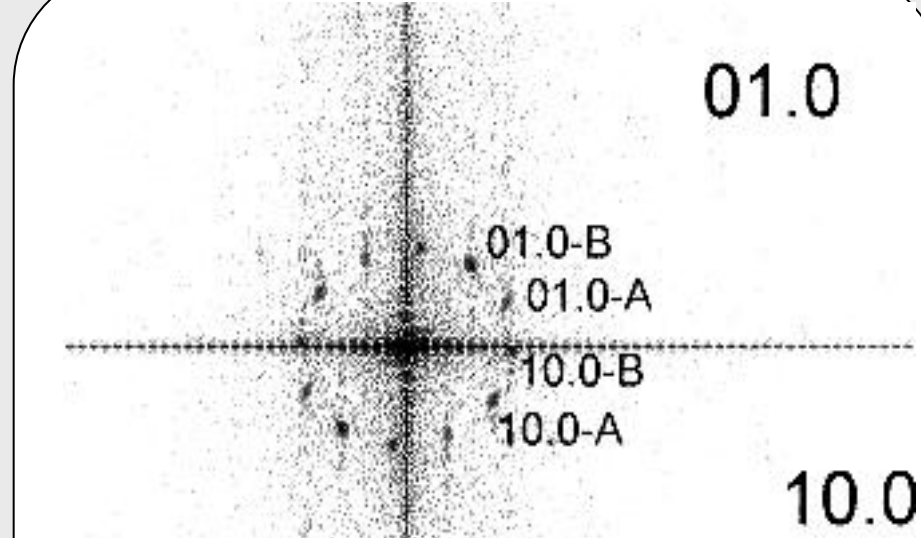
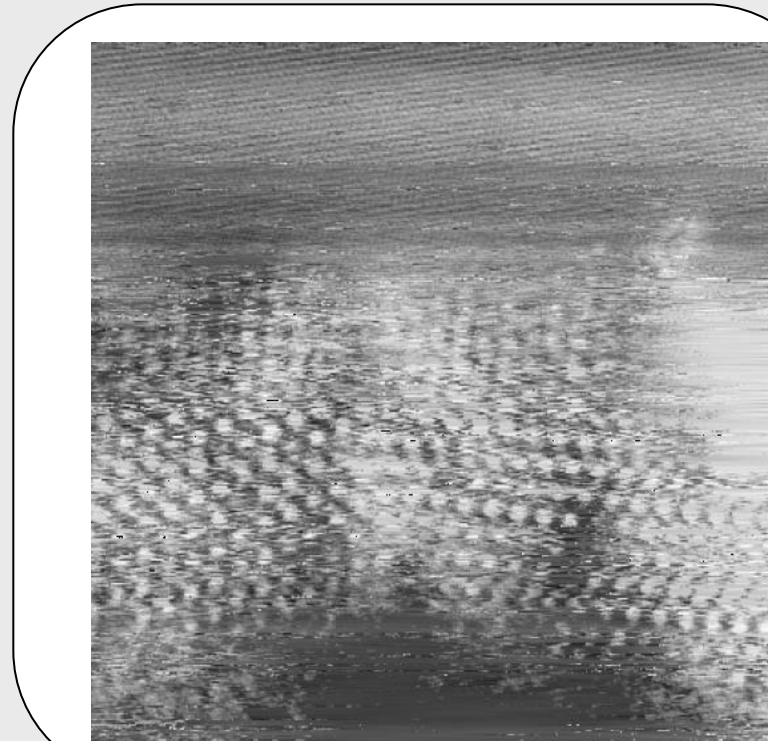
STM images of the surface of NbSe₂



The undistorted (001) surface (10 nm)² of NbSe₂

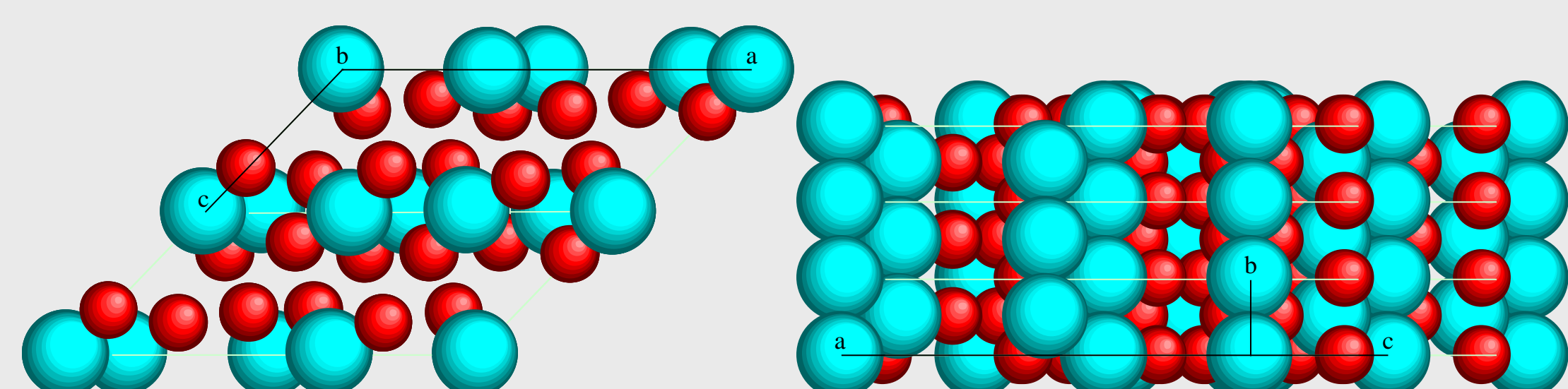


Missing Se-Nb-Se disc (left), magnified area (30 nm)² with modulation domains (right) of the $\sqrt{3}a_0 \times \sqrt{3}a_0$ phase



Fast Fourier transform of the area shown in the middle (two variants)

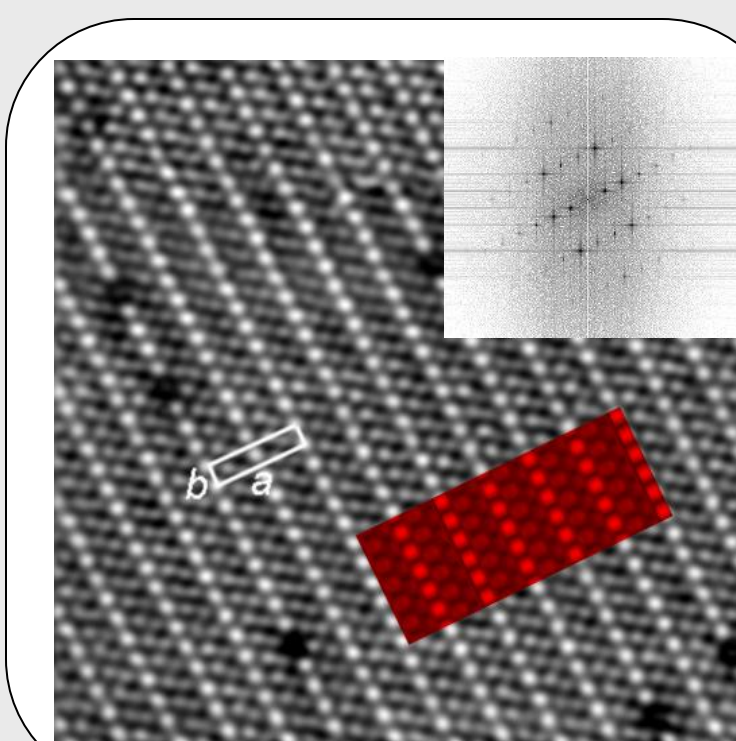
The basic structure of NbTe₂



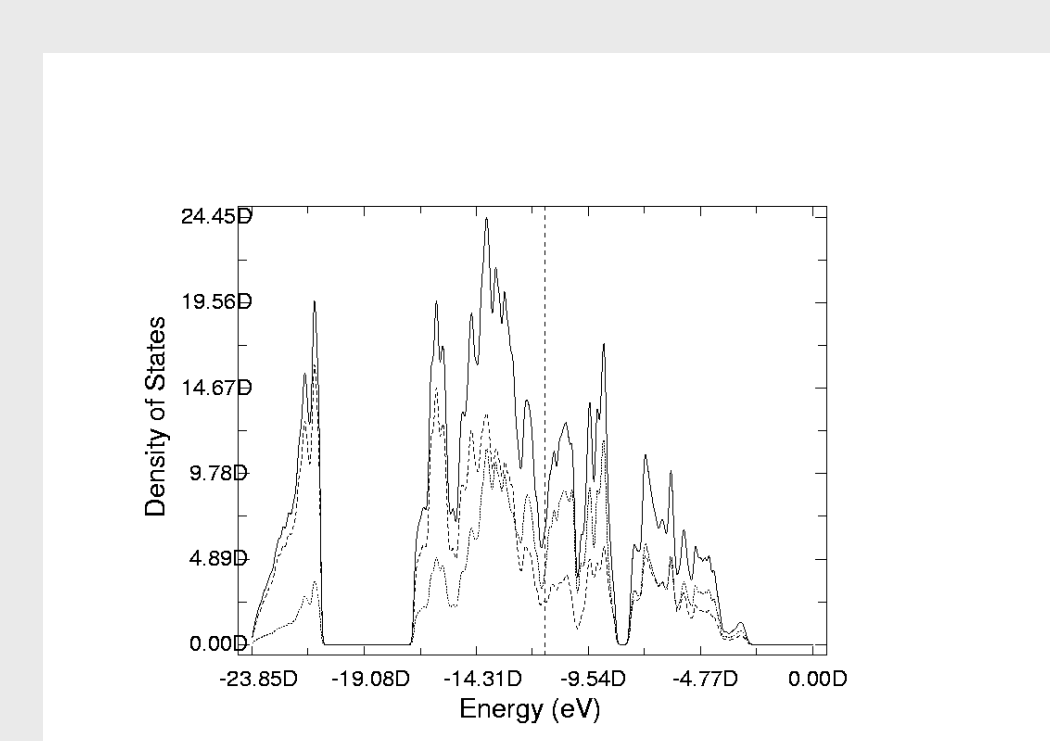
Te
Nb

SG : C2/m, deformed CdI₂ - type;
a₀, b₀, c₀ = setting of CdI₂
a=3√3a₀=19.39 Å b=a₀=3.642 Å c=c₀/sinβ=9.375 Å
β=134°35'

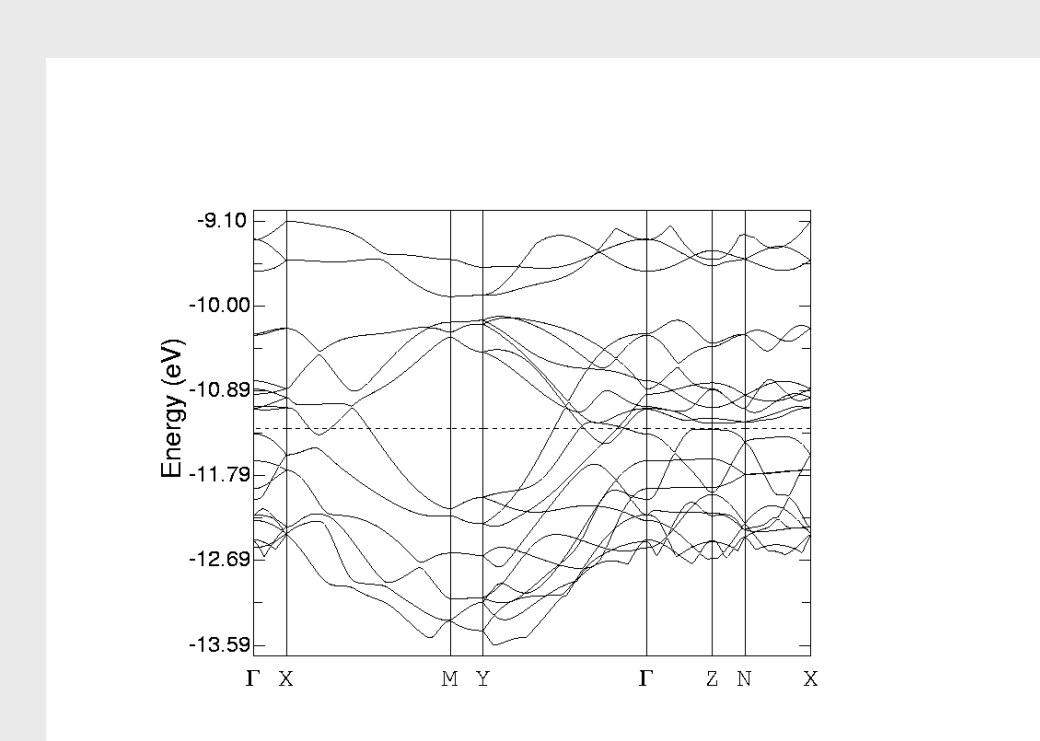
TM and calculated electronic properties of NbTe₂



STM image of a cleaved (001) surface

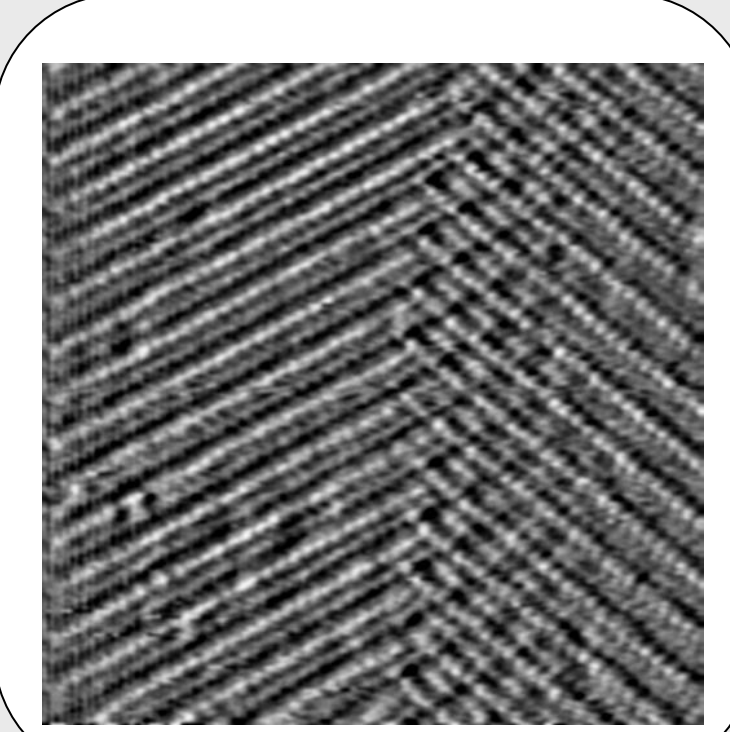
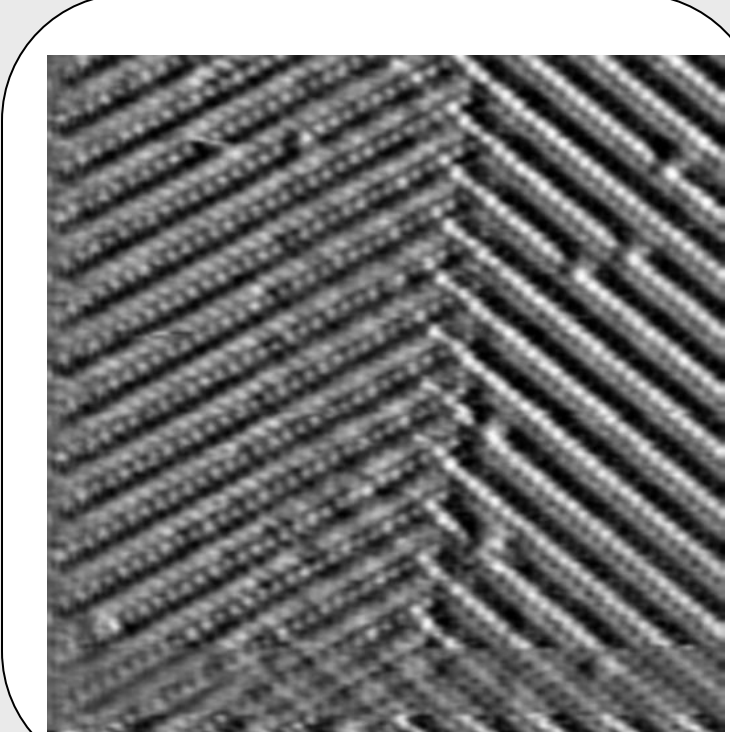
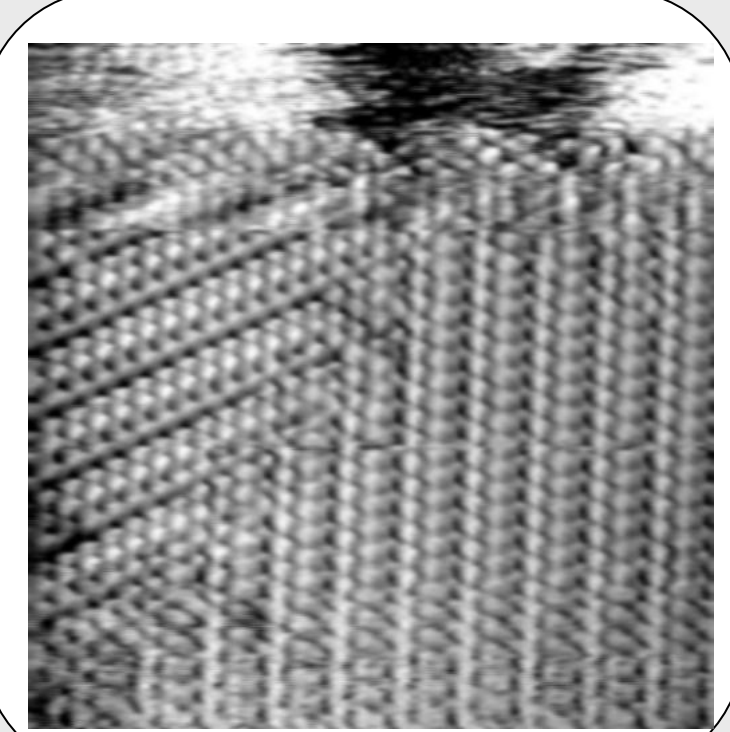


Density of states calculated by the EHTB-method



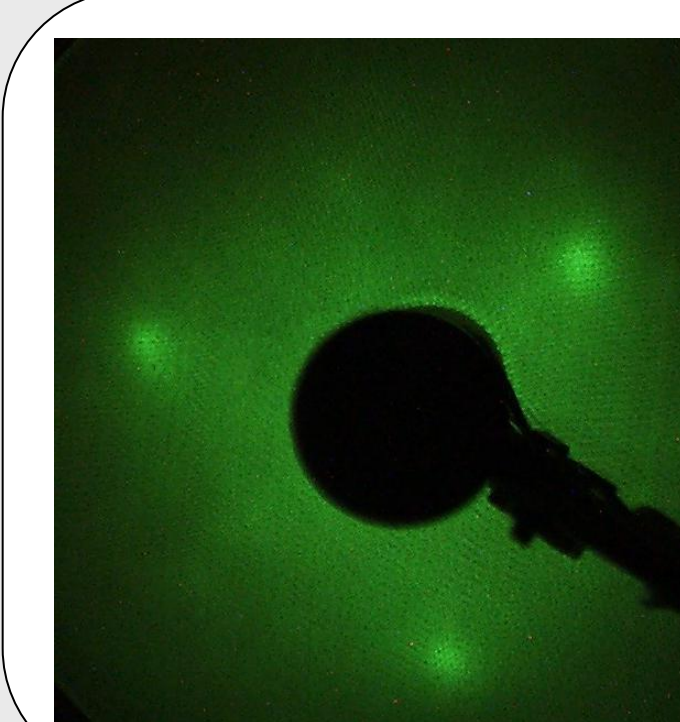
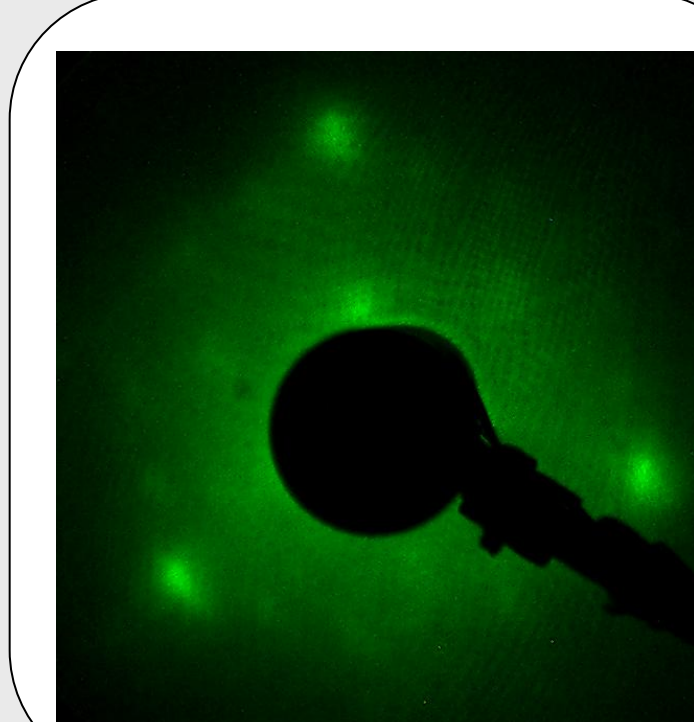
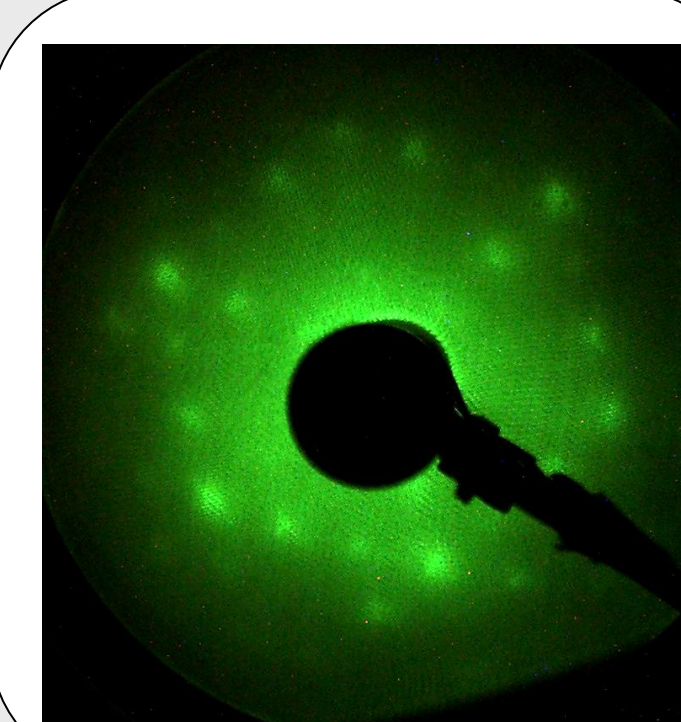
Dispersion curves calculated by the EHTB-method

Domain boundaries in NbTe₂



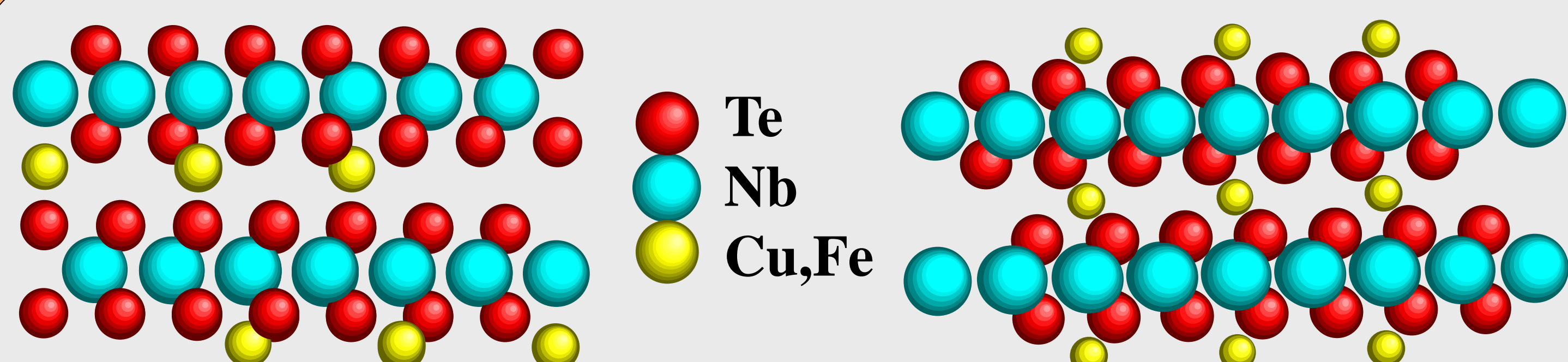
Domain boundaries formed due to a collapsed CdI₂ structure.
Two orientational variants, 60° (left) and 120° (middle), the same area as the picture in the middle scanned a few seconds later (right)

Low energy electron diffraction of NbTe₂



LEED as a function of the electron energy 80 eV (left), 89 eV (middle) and 113 eV (right)

Intercalated NbS₂

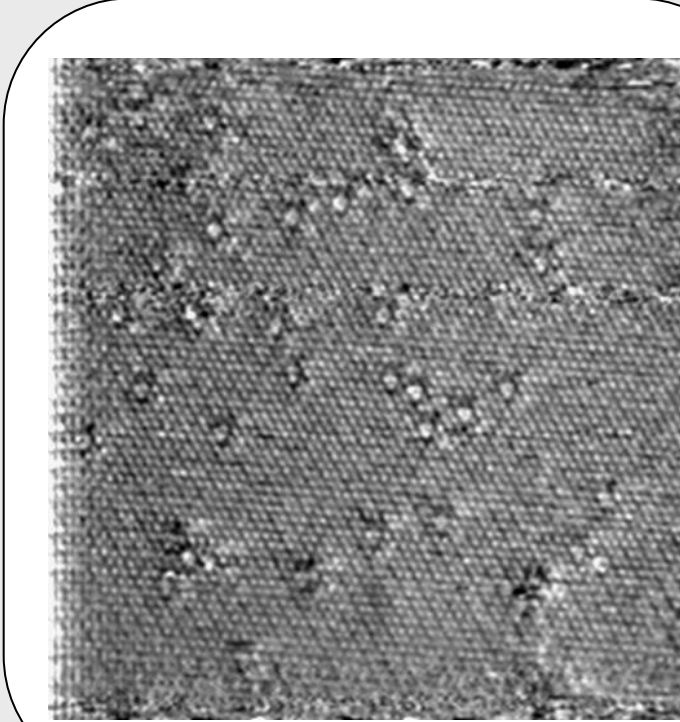


Te
Nb
Cu, Fe

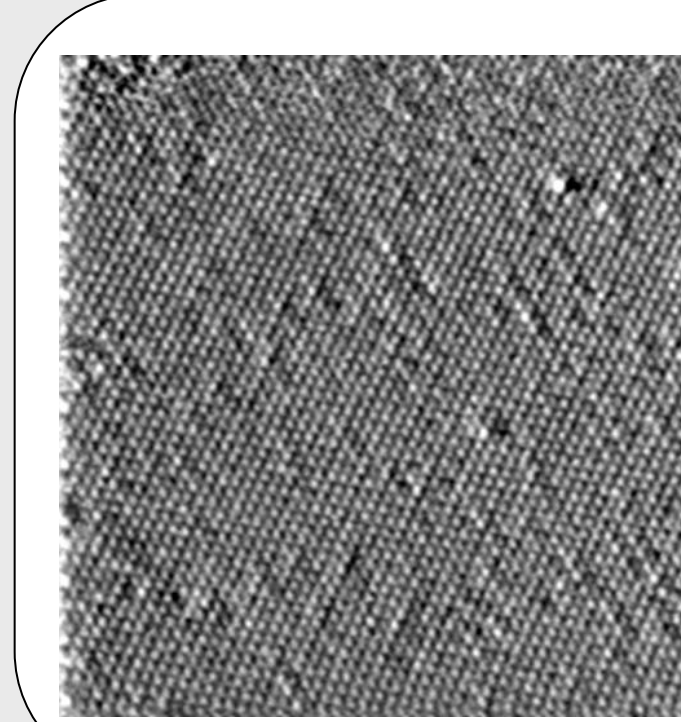
Intercalation with Cu:
The 2H_b-MoS₂ polytype is formed
Cu in tetrahedral interstices

Intercalation with Fe or Co:
The 2H_a2NbS₂ polytype is formed
Fe or Co in octahedral interstices

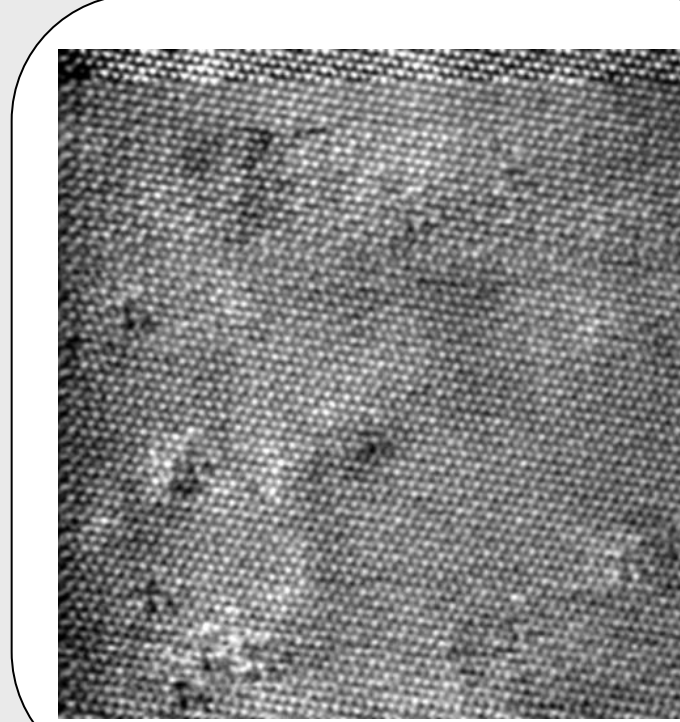
Superstructures formed by intercalation



2a x 2a hexagonal superstructure in Fe_{0.25}NbS₂ at room temperature



partly ordered 2a periodicities in Cu_{0.33}NbS₂ at room temperature



$\sqrt{3}a \times \sqrt{3}a$ superstructure in Co_{0.33}NbS₂ at room temperature