



The Domain Structure of NbTe₂

D. Cukjati¹, A. Prodan^{1*}, N. Jug¹, H. J. P. van Midden¹, P. Starowicz¹, H. Böhm²,

F. W. Boswell³ and J. C. Bennett⁴

¹Institute Jožef Stefan, Jamova 39, SI-1000 Ljubljana, Slovenia ²Geowissenschaften, Johannes Gutenberg Universität, D-55099 Mainz, Germany ³Department of Physics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1 ⁴Department of Physics, Acadia University, Wolfville, Nova Scotia, Canada B0P 1X0

*the corresponding author: albert.prodan@ijs.si







TEM/TED of the domains









SG : C2/m , deformed CdI₂ – type; $a_0, b_0, c_0 = setting of CdI_2$ $a=3\sqrt{3}a_0=19.39$ Å $b=a_0=3.642$ Å $c=c_0$ /sinß=9.375 Å ß=134°35'

Only ortho- and meta-boundaries are imaged with the beam along the [001]* direction. The (103)* section through the reciprocal reveals space the corresponding twin planes.



Strain is often released by mutually orthogonal domains of irregular shapes, formed of meta polysynthetic twins.

By heating the sample with the electron beam the parent CdI_2 structure is formed (a), occasionally accompanied by a pronounced incommensurate modulation (b).

STM of the surface and of the domains



Variation of the STM image with the tunnelling current.





a) $(20nm)^2$, CCM, U_a=-0,1mV, I_t=0,8nA, t=300µs, Pt-Rh tip b) $(10nm)^2$, CCM, U_g=0,1mV, I_t=2nA, t=400µs, Pt-Rh tip c) (10nm)², CCM, U_q=0,1mV, I_t=40nA, t=400µs, Pt-Rh tip



A coherent ortho twin boundary (60° between the unit cells, 120° between the corrugation lines) (a), a coherent meta twin boundary (reversed angles) (b) and APBs aligned along the scanning direction (c).

a) $(20nm)^2$, CHM, U_a=0,1mV, I_t=3nA, t=30µs, W tip b) (20nm)², CHM, U_g=0,1mV, I_t=3nA, t=30µs, W tip c) (20nm)², CHM, U_g=0,1mV, I_t=3nA, t=30µs, W tip



Three domains in contact. The boundaries are either stepped (a) or irregular (b) and the adjacent regions are often modulated.

a) (20nm)², CHM, U_g=0,1mV, I_t=3nA, t=30µs, W tip b) (15nm)², CHM, U_g=0,1mV, I_t=4nA, t=30μs, W tip

The variation of an ortho-boundary with subsequent scanning. A strongly modulated boundary (a), sharpened with a step reaching the edge of a modulated region (b), straightened with a remaining single-atom-step (c) and finally fully straightened (d). The modulation corresponds to the periodicity of the adjacent domain.

 $(15nm)^2$, CHM, U_g=0,1mV, I_t=3nA, t=30µs, W tip

Electronic properties and STM simulation

LEED of the surface





(12nm)², CCM, U_q=0,1mV, I_t=3nA, t=6µs, W tip

E = 100 eVE = 89 eVE = 80 eVVariation of the LEED pattern with electron energy. Above about 90 eV only reflections from the CdI_2 structure are observed. All reflections are weak and diffuse. E = 113 eVE = 166eV

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