Motivation: DiMe-PTCDI on alkaline halide (001) surfaces

Topic of interest: growth of organic molecules on insulating surfaces (→ molecular electronics, ...)

Model system:
- Alkali halide(001) surfaces, easy to prepare
- Prototypical organic semiconductor molecules (C₆₀) [1], PTCDA [2, 3]

BUT: no “controlled” growth so far: e.g. on KBr(001): \( C₃₀ \) (fractal islands), PTCDA (3d crystallites)

New candidate: DiMe-PTCDI

Technique: frequency modulation (FM) → AFM

- Sample is brought near an oscillating silicon cantilever with tip
- Tip-sample forces change the resonance frequency, distance control keeps the frequency shift of constant: atomic resolution imaging also on insulating surfaces possible
- Second control loop keeps amplitude constant: external driving energy = dissipated energy

Experimental details
- Experiments performed in UHV
- Microscope: Omicron AFM/STM in non-contact → mode (@ 300 K)
- Sample preparation: KBr(001)/NaCl(001) single crystals (Korth, Germany) in situ – cleaving
- Heating to 450 K after cleavage
- Evaporation of various amounts of DiMe-PTCDI from home-built crucible (sample @ 300 K)
- Flux control: quadrupole mass spectrometer

Experiments: DiMe-PTCDI on KBr(001)

Low coverage:
- Molecules form long “wires”: < 10 nm wide, 600 nm long
- Wires stretched over substrate terraces
- Pinned at step edges
- Not stable otherwise?
- Between wires: atomic resolution of KBr, no wetting layer of molecules

Higher coverage:
- More wires, at least 2 molecular layers high
- Wires stretched between step edges or between other wires
- Preferred orientation: along substrate [110] direction
- Too narrow to scan upon a wire → no molecular resolution

No step edges around?
- Well-cleaned KBr crystal, huge terraces (µm)
- Scans ~ 10 min after evaporation of molecules
- Wires move or vanish → high mobility of molecules on the surface

Evaporation on cold crystal (~250 K)
- Height of wires: one layer
- KBr step edges determine the orientation
- Wires as short as possible between steps
- Both [110] and [110] occur when neither direction is preferred by step edges
- KBr steps break into [100] and [010] kinks; kinks might act as nucleation centers
- No molecular resolution possible (sample heating up!)

Model: force field calculation + common sense
- Interaction: empirical potential (AMBER) + electrostatic interaction
- Results: optimum position for a single molecule
- [110] preferred, on top of Br ion
- Preferred orientation + close-packed arrangement = wire

Tentative Model:
\[ p(2 \times 2) → \text{superstructure on KBr(001)} \]
(see also [5])

New Experiments: DiMe-PTCDI on NaCl(001)
- Wires on KBr unstable (obviously);
- Desirable: more stable wires
- General mechanisms?
- NaCl lattice constant 563 pm (KBr: 658 pm)
- \( p(2 \times 2) → \text{superstructure on KBr: not sooo close-packed} \)
- Molecules form “wires”, 2 ML high, [110] direction
- Wires stretched over substrate terraces, not pinned at step edges
- Shape of wires does not change for several hours
- Between wires: atomic resolution of NaCl

References

Acknowledgement
Financial support is granted by the Deutsche Forschungsgemeinschaft (DFG) through SFB 616 “Energy dissipation at surfaces”

Contact
Manfred Lange
Tel.: +49 203 379 2137
manfred.lange@stud.uni-due.de

Prof. Dr. R. Möller
Tel.: +49 203 379 4220
rolf.moeller@uni-due.de

SFB 616
organic-molecular-nanowires

SFB 616
Organic Molecular Nanowires: The growth of DiMe-PTCDI on KBr(001) and NaCl(001)
M. Lange, M. Fendrich, C. Weiss, T. Kunstmann, and R. Möller

Fachbereich Physik und Center for Nanointegration Duisburg Essen (CeNiDE), Universität Duisburg-Essen, D-47048 Duisburg