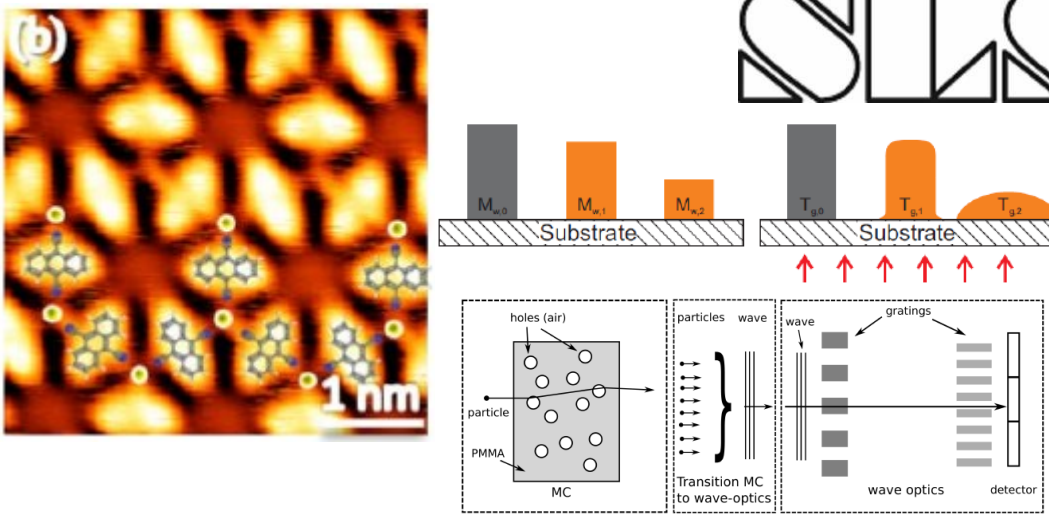

SLS Symposium on

Soft Matter

Tuesday, April 7, 2015

10:00 to 11:45, WBGB/019

10:00 Numerical simulation of phase-sensitive X-ray imaging using Monte Carlo methods
Silvia Peter, P. Modregger, M. K. Fix, W. Volken, P. Manser and M. Stampanoni

10:30 Thermal polymer reflow: Energy-based geometry evolution and 3D simulation
Robert Kirchner and H. Schift

11:00 Coffee

11:15 Interaction of electronic states in metal-coordinated and hydrogen bonded molecular networks on Cu(111)
Jun Zhang, A. Kara, T. A. Jung, and M. Muntwiler

Numerical simulation of phase-sensitive X-ray imaging using Monte Carlo methods

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Hard X-ray grating interferometry (GI) is a recently established phase sensitive imaging technique with the advantage of simultaneously providing three complementary types of contrast: absorption, phase and dark-field contrast [1]. GI phase contrast and dark-field imaging have a wide range of possible applications in medical diagnostics and biomedical research [2]. In addition, it has been shown that sub-pixel structure information of a sample can be obtained trough ultra small-angle X-ray scattering (USAXS) [3].
However, there are still open questions remaining about the details of the contrast formation process, such as the link between the measured scattering signal and the physical properties of a sample in dark-field and USAXS imaging.
A convenient method to obtain a deeper understanding of the image formation process is through numerical simulations. Since phase contrast relies on beam coherence and dark-field contrast relies on scattering, both particle-like and wave-like properties of X-rays have to be considered within a realistic simulation of the contrast formation mechanism. On the one hand wave-optics simulations are a well suited method for simulating coherent effects such as phase-shift and interference, but scattering cannot be modeled in a straight forward way. Monte Carlo methods (MC), on the other hand, are a convenient way to model scattering and absorption but wave-like properties such as interference are neglected.
A simulation framework that combines MC with wave-optics for a realistic simulation of both particle-like and wave-like behaviour of X-ray in imaging has been developed [4] and the results of the simulations performed with this model were used for the development model for the description of the connection between he obtained signal and the physical structure of the sample in GI USAXS. This is of great importance for a quantitative evaluation and interpretation of the obtained image.

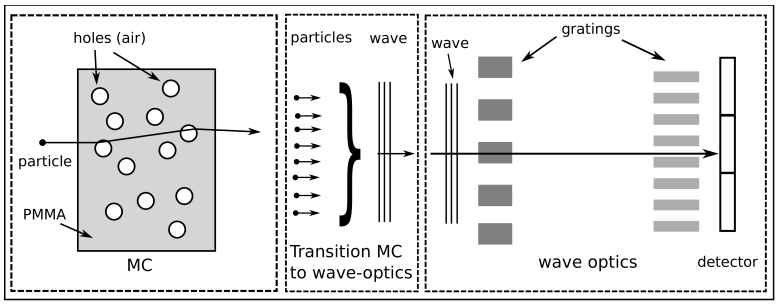

Figure 1: Sketch of the simulation framework

References

[1] A. Momose et al, Japanese Journal of Applied Physics, 42, 2003

[2] S. McDonald et al, Journal of Synchotron Radiation, 16, 2009

[3] P. Modregger et al, Physical Review Letters, 108, 2012

[4] S. Peter et al, Journal of Synchotron Radiation, 21, 2014

Thermal polymer reflow: Energy-based geometry evolution and 3D simulation

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The ability for 3D manufacturing is crucial for future fluidic and photonic devices. Polymer patterning techniques are promising for such applications due to a broad spectrum of available polymers, the ability for efficient tuning of their properties and the usability of respective emerging technologies. For example, electron beam grayscale lithography has demonstrated its potential for multi-tier structures down to the nano-scale.[1] Polymer reflow has recently proven its ability to transform such multi-tier structures into complex convex and concave patterns on the micro-scale.[2] The manufacturing of complex 3D patterns by combining these two approaches (Fig. 1) requires a high predictability for the final reflow geometry. This work discusses the main reflow effects (e.g. Fig. 2) and their implementation in an energy-based simulation approach (Fig. 3). For the latter, the free software Surface Evolver[3], being based on a minimal-energy soapfilm-method, was used.

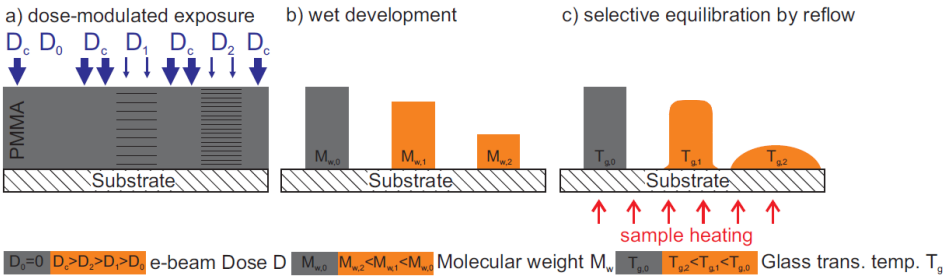

Fig. 1: Schematic of the process flow combining electron beam grayscale lithography and polymer reflow for selective pattern equilibration.

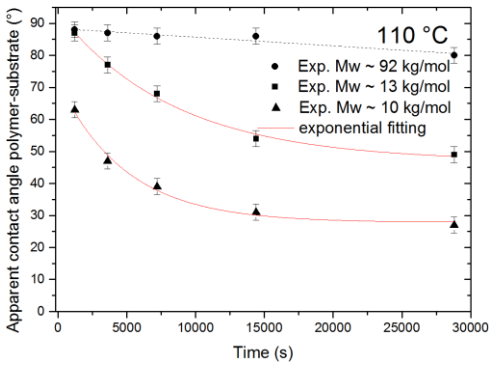

Fig. 2: Evolution of the apparent contact angle

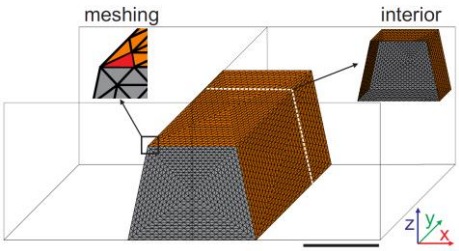

Fig. 3: Initial geometry for a reflow simulation of a single line demonstrating the triangular meshing and the soapfilm-approach.

[1] F. Hu and S.-Y. Lee, J. Vac. Sci. Technol. B (26) 2003, pp. 2672-2679
[2] A. Schleunitz and H. Schift, J. Micromech. Microeng. (20) 2010, pp. 095002
[3] K. A. Brakke, Experimental Mathematics (1) 1992, pp. 141-165

Interaction of electronic states in metal-coordinated and hydrogen bonded molecular networks on Cu(111)

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The metal/molecule interface, important to organic-based electronic and optoelectronic devices, represents a unique system in which extended metallic states interact with molecular networks or localized molecular states.

The goal of this study is to understand the interplay between the geometric and electronic structures at the interface between organic semiconductor molecules and metal substrates by using scanning tunneling microscopy (STM) and X-ray photoelectron diffraction. We use 9, 10-dicyanoanthracene (DCA) molecule on Cu(111) as a model system, which forms various self-assembled structures under controlled evaporation conditions. As shown in Figure 1, DCA molecules can be fully or partially coordinated with Cu adatoms (Figure 1(b), or (c)) via the CN function group. The molecules can also form single or double molecular lines with hydrogen bond interaction (Figure 1(d) and (e)). In these structures, we observe different electronic states, such as confined states derived from the Shockley surface state, an interface state and a hybridized molecular state with adatoms. For example, due to the porous structure of the metal coordinated network, the surface state is confined to a series of discrete states. Energy and momentum of these states are related both to the energy dispersion of the free surface state and the electronic potential landscape of the network. On the other hand, the interaction between molecule and substrate can also strongly influence the molecular electronic state, especially in cases where adatoms are involved. In hydrogen bonded structures, an interface state appears which cannot be clearly attributed to either the molecule or the substrate. Likewise, the coupling between the molecular orbital and the electronic state of the Cu adatom forms a hybridized state, which interconnects the molecules in the network electronically.

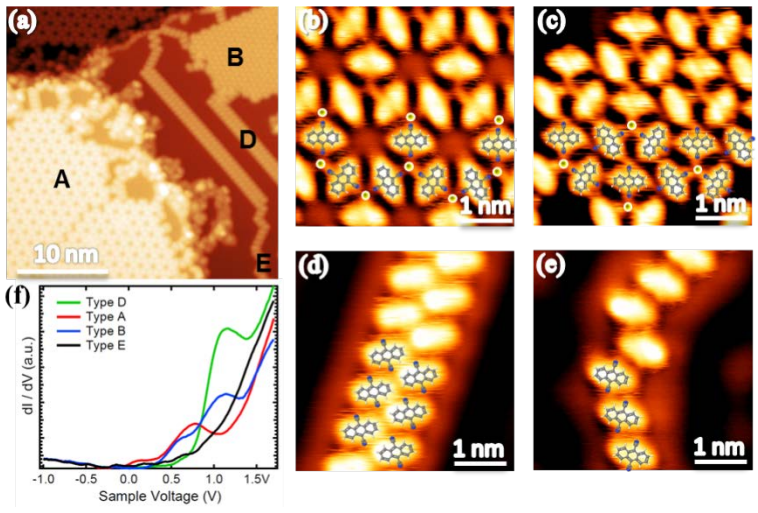

Figure 1 (a) STM image (-1.0 V, 20 pA, 30 nm × 30 nm) of DCA molecules on Cu(111), which shows different molecular assembly structures as marked. (b-e) High resolution STM images (-0.5 V, 50 pA, 4.2 nm × 4.2 nm) for structures A, B, D and E, respectively. The proposed structure model is superimposed. (f) dI/dV spectra obtained in the center of molecules in different structures shown in (b-e).