Übungen zur Oberflächenphysik Blatt 3 – 02.4.2013

1) Surface Diffusion

- a) The hopping rate of a nitrogen atom on the Fe(100) surface is 10^{-3} s⁻¹ at 300 K and $3x10^{-2}$ s⁻¹ at 330 K. Estimate the diffusion coefficient and calculate the activation energy. Take into account that Fe is a bcc crystal with lattice parameter 2.87 Å. Assume the vibration frequency n₀ is $4.3x10^{12}$ Hz.
- b) Random-walk diffusion of Ag atoms occurs over the Si(111) $\sqrt{3x}\sqrt{3}$ -Ag surface. Estimate the mean displacement of the atom in a time of 1 s and 1 h at 450°C. D₀ = 10⁻³ cm²s⁻¹, E_{diff}=0.33 eV.

2) Thin film growth

a) Thermodynamics



- i) Name the three growth modes shown above.
- ii) Explain why a film grows on a substrate in each of the growth modes using the surface tensions.
- iii) How can you experimentally distinguish the three growth modes using XPS?
- iv) How can you distinguish them with RHEED?

b) Kinetics

The film is grown homoepitaxially by Molecular Beam Epitaxy MBE process. The Knudsen cell is L=5cm from the substrate and area of the

substrate is a=0.5 cm². Estimate to what temperature we need to heat the cell to obtain growth rate of 1 μ m/h for Ga material?

3) LEED a) Simple LEED pattern

Assume that you found the following LEED pattern, measured on a Cu(001) substrate and Cu(111). The white circles correspond to the substrate surface¹ and the crosses correspond to domains of the adsorbate².

a)	o	o	o	0	b)	٥	×	×	0	×	x	٥	c)		0	×	0	
- · ,	x	x	x	x	-	×			×			x X			×	~	x	
	o	o	ο	0		0	×	x	0	×	x	0		0	×	0	x	0
	x	×	×	×		x			×			××				x		
	ο	ο	0	0		ö	×	x	õ	x	×	õ			o		0	

- i) Reconstruct the real lattice for the a) and b) and c) adsorbate domains.
- ii) Find the Wood and Matrix notation
- b) Complex LEED pattern



- i) The figure above shows real data of a big quadratic molecule (MnTPPCI) self-assembled on Ag(111). The LEED pattern is already solved (reciprocal space: fig. *b*, real space: fig. *c*), you just have to find the Matrix notation (fig. *c*: adsorbate unit cell: black arrows, substrate: green arrows).
- ii) The above example shows that a 3-fold substrate where a quadratic molecule is assembled in 3 *rotation domains*. Briefly reflect on this fact, i.e. what about rectangular molecules, chiral molecular adsorbates?

¹ experimentally deduced by a reference measurement

² experimentally sometimes concluded from intensity fluctuations upon lateral movement of the sample, generally not so easy

4) RHEED

RHEED intensity oscillations are frequently used to monitor the epitaxial growth of heterostructures for applications in micro- and opto-electronics.

a) Calculate coherence length of the RHEED. The angular width of beam is 10^{-2} rad and energy spread is 250 meV at standard energy of the RHEED beam E=5 10^4 eV.



b) Demonstrate the sub-monolayer sensitivity explaining the nature of the oscillations during the epitaxial monolayer growth, i.e. what happens in the intensity minima and maxima? Explain.