Single molecule in a tip-surface junction: Modeling and calculations in the context of non-contact AFM

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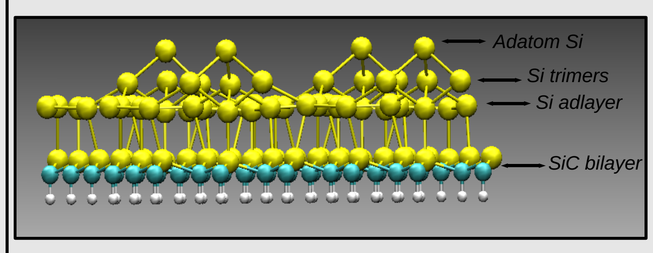
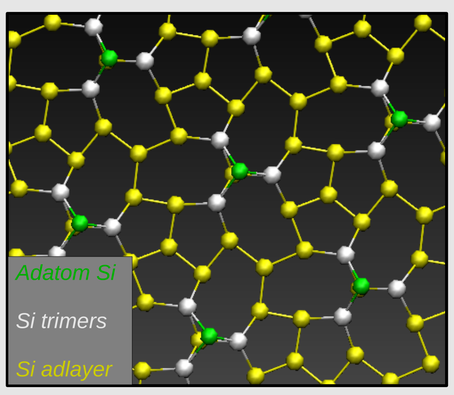
Context of the ANR MOLSiC project

☼ Substrate with a large band gap as silicon carbide (SiC) is chosen.
☼ STM study at low temperature is difficult without specific dopping. Frequency-Modulation nc-AFM is thus well adapted for the study of surface properties of SiC.
☼ In a first stage, modeling of the nc-AFM setup and simulations of its behaviour have been performed.
☼ This contribution of the MolSiC project is included in a consortium involving experimentalists of CEMES (Toulouse), IM2NP (Marseille), ICMO (Orsay) and theorititians of IS2M (Mulhouse).

SiC surface

☼ Silicon carbide is supposed to play an important role in electronics with high power, at high temperature and high frequency.
☼ Numerous surface reconstructions have already been determined and offer many intrinsic properties.
☼ The consortium focuses on one of these reconstructions that is the 6H-SiC (0001) 3x3.





Distance between two adjacent adatoms ≈ 9,30 Å

Suitable force field for silicon carbide

☼ Empirical interatomic potentiel :

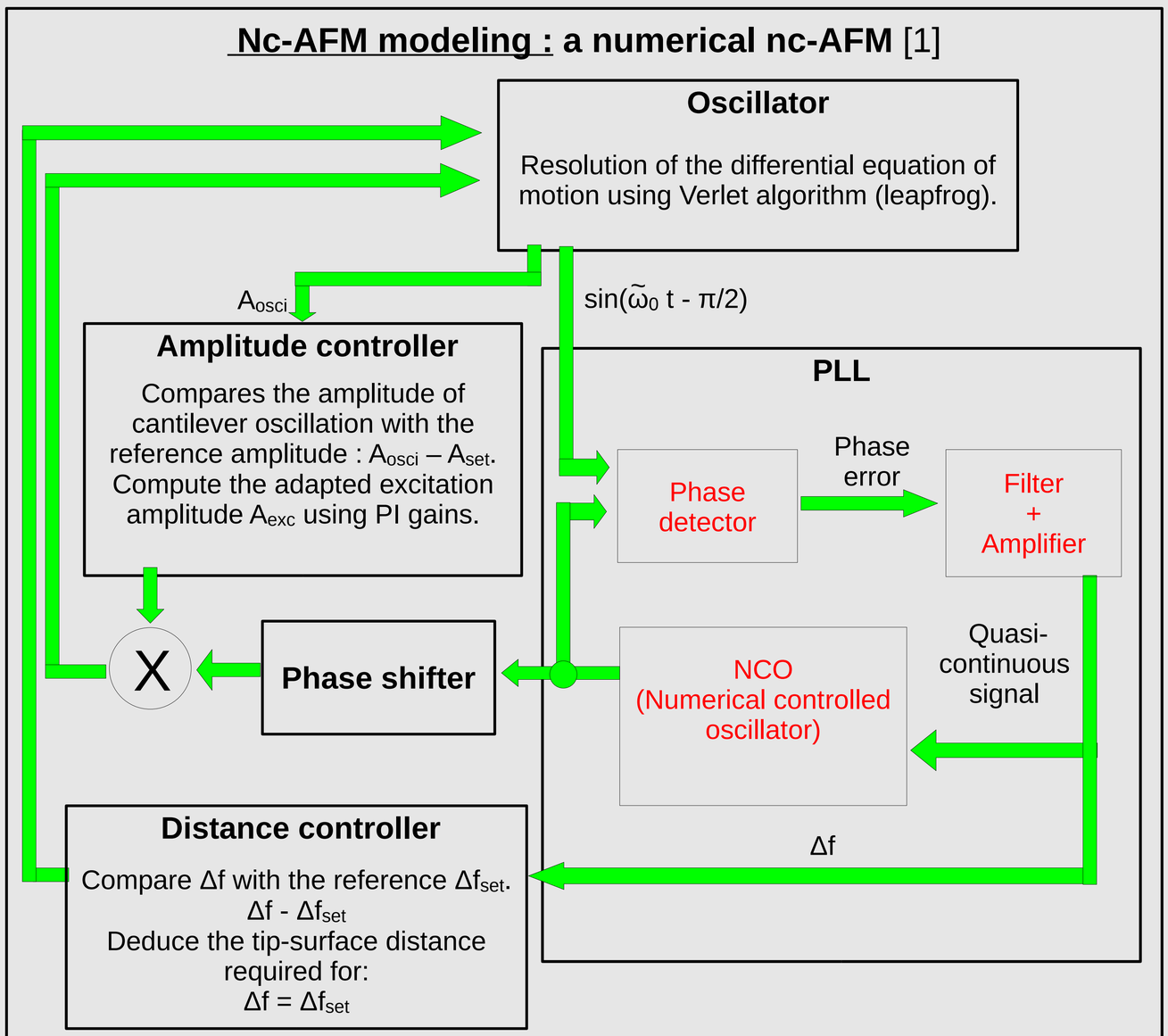
$$E_V^{i-j} = \epsilon\,(1.84 * 10^5 \exp^{-\frac{12}{P}} - 2.25P^6)$$

$$avec \quad \epsilon = \sqrt{\epsilon_i \epsilon_j} \quad et \quad P = \frac{r_i + r_j}{R}$$

☼ ϵ_i, ϵ_j = Hardness of atoms i et j (kcal/mole).

☼ r_i, r_j = van der Waals radii of atoms i and j (Å).

Nc-AFM modeling : a numerical nc-AFM [1]



[1] L.Nony, A.Baratoff, D.Schär, O.Pfeiffer, A.Wetzel and E.Meyer, Phys. Rev. B **74**, 235439 (2006)

First results

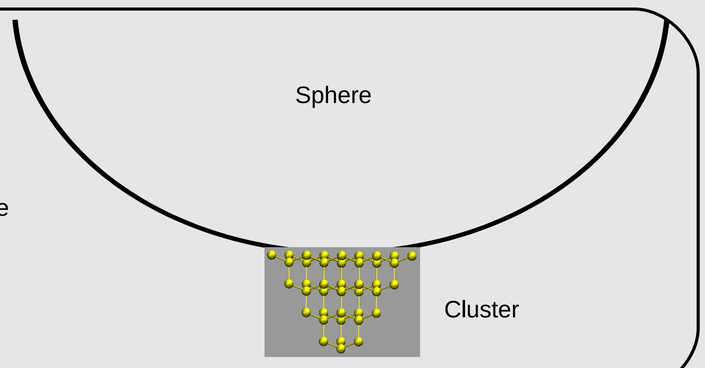
☼ *Details about numerical nc-AFM:*

- The numerical nc-AFM is able to be used at large amplitude and at small amplitude, mimicking the **Qplus** setup.
- It can generate the topographic data set by operating in one of two modes: **constant-height** or **constant-Δf** mode.

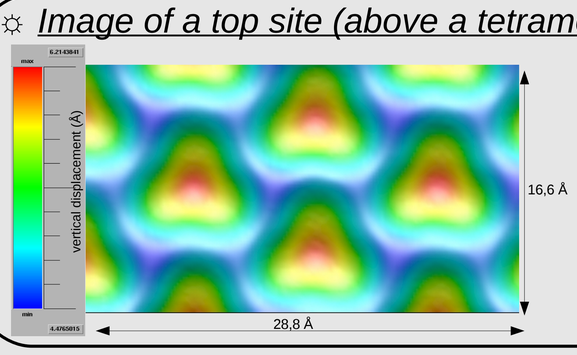
☼ *Description of the tip:*

Sphere:
- radius = 40 Å

Cluster:
- diamond-like structure
- 54 Si atoms
- height = 10 Å
- full tip angle = 70°



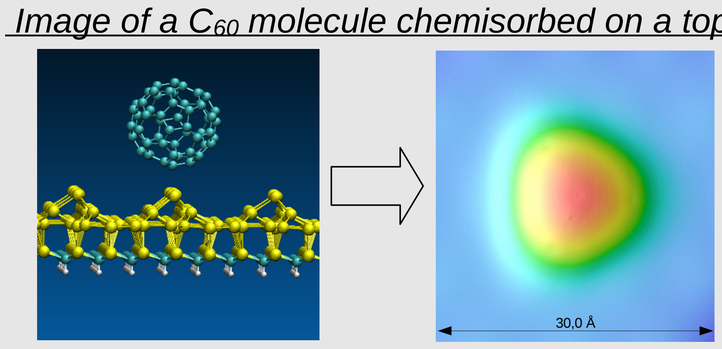
☼ *Image of a top site (above a tetramer) of SiC at constant Δf:*



Qplus parameters:
- f_0 = 23165 Hz
- Q = 50000
- k_c = 1800 N.m^{-1}
- A = 0,2 Å
- Δf_set = -150 Hz

Observation:
- Maximum corrugation = 1,83 Å

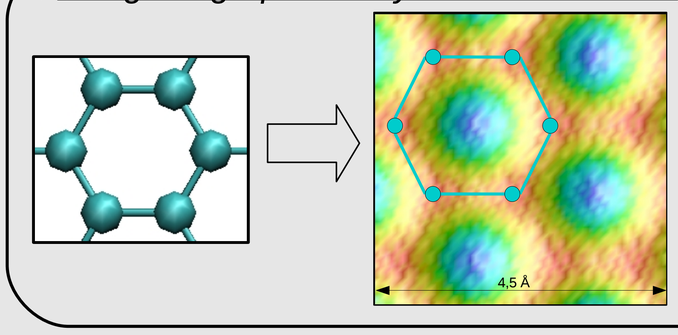
☼ *Image of a C_{60} molecule chemisorbed on a top site of SiC:*



Parameters:
- f_0 = 150 kHz
- Q = 30000
- k_c = 40 N.m^{-1}
- A = 100 Å
- Δf_set = -50 Hz
- V_{scan} = 2 Å.s^{-1}

Observations:
- Corrugation max = 6,6 Å
- Diamètre = 19 Å

☼ *Image of graphene layer at constant height:*



Qplus parameters:
- f_0 = 23165 Hz
- Q = 50000
- k_c = 1800 N.m^{-1}
- A = 0,2 Å
- h = 3,52 Å

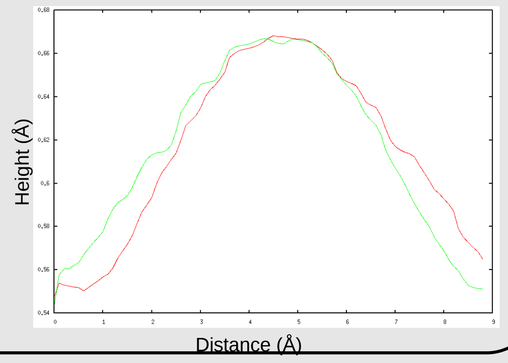
Observation:
- Maximum corrugation = 0,7 Hz

☼ *Tip effects:*

Scan above a SiC pyramid:

Green: with an edge of the tip.

Red: with a facet of the tip (rotation of 30° according to the z axis).



Outlook:

☼ Calculation of relaxed functionalized molecules on a SiC surface by using molecular mechanics like procedure.

☼ Study of their behavior when interacting with an AFM tip during scanning by introduction of molecular dynamics in the numerical code.