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Atomic Force Microscope Functionality Simulation: Physical and Energetic Analogies

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Using Atomic Force Microscopes (AFM) to manipulate nano-objects is an actual challenge for both physicians and biologists. Many visual and haptic interfaces between the AFM and experimentalists have already been implemented. The multi-sensory renderings (seeing, hearing, feeling) studied from a cognitive point of view increase the efficiency of the actual interfaces and represent our challenge. To allow the experimentalist to *feel and touch* the nano-world, we add mixed realities between an AFM and a force feedback device, enriching thus the direct connection by a modeling engine. The functionality of an AFM is described in this paper through physical and energetic analogies.

Firstly, we present a physical model, able to be simulated in real time that allows user to feel in his fingers and act on the virtual scene of a nano-world. The existing force between the AFM tip and the nano-surface in a cohesive interaction is transmitted to the experimentalist in real time through the designed model and the Force Feedback Gestural Device, making thus possible a human haptic perception of the approach-retract interaction. This minimal representation of the real and complex phenomenon of approbation interaction is then strengthened and validated by an electro-mechanical model, through which we integrate functional AFM components in a Simulink model.

Secondly, we describe the same interactions from the dual energetic point of view. This representation enriches the force feedback rendering with a visual perception of the phenomenon. Therefore, the presented models and their results match the physical experiments and improve the existing interfaces by taking in account the full cognitive capabilities of the user.

By means of the Cordis-Anima modeling and simulation system, a minimal representation of the real and complex phenomenon of approach-retract interaction is created. The components involved in this interaction: the piezo element, the tip and the sample surface are modeled like material objects with their specific weights and inertias, that are permanently in interaction with the external environment as well as among them. The equivalent schema is presented in fig. 1, where the cantilever is represented as a spring with zero length in vide and driving the tip on the Oz axis, while the tip-surface interaction is treated as a non-linear interaction.

The results of this minimal model are illustrated in the figures numbered from 1 to 8 on the left side of the poster. When the tip approaches to the surface (fig.1 to 4), attractive forces appear and act on the tip being transmitted also to the cantilever according to the action-reaction principle. The spring ensemble and the non-linear tip-surface interaction determine the sudden approach of the tip to the surface which is followed by a relaxation of the spring that model the cantilever, and is due to the piezo element position descending. On the opposite sense (fig. 5 to 8), when the tip retracts from the surface, the forces involved are stronger then in the approach phenomenon that explains the longer spring elongation. The tip position tends to become the piezo element position and the interaction forces tend to zero. After a spring compression that corresponds to the tip separation from the surface, a relaxation without oscillations due to the defined stiffness of the system formed from piezo element-cantilever-tip at the equilibrium position occurs.

The existing force between the AFM tip and the nano-surface in this cohesive interaction is transmitted to the experimentalist in real time through the designed model and the Force Feedback Gestural Device (figures on the left side, at the bottom of the poster). Thus, the user has a haptic perception of the approach-retract interaction being able to feel the force intensity: lower at approach moment and stronger at retract moment.

In order to obtain a confirmation of this minimal representation of the approach-retract phenomenon, we developed an electro-mechanical model (figure on the right side of the poster) for the ensemble piezo element – cantilever – tip and its interaction with the sample surface. The functional point of the AFM system during the approach-retract phenomenon is the cross-point between the tip characteristic curve resulted from Lennard-Jones potential and the cantilever characteristic curve. Analyzing the AFM functionality from this point of view, an approach-retract interaction curve with its typical hysteresis is obtained.

In order to enrich the force feedback rendering with a visual perception of the approach-retract phenomenon, we describe the same interaction from the energetic point of view. Thus, interaction force curves are treated in the following in terms of potentials. The AFM system functionality is represented by the sum of surface potential and tip potential.

The equilibrium position of the tip in the total potential (the sum of the two potentials: electric and Lennard Jones) is well determined at each tip-surface distance. In the numerical simulation of the approach-retract interaction, the tip is treated as a punctual object, while the surface is an infinite semi-plan. The surface is considered very rigid comparing to the tip. The computational results are presented in terms of a total potential but the real calculation is done in force terms: the Van der Waals and the cantilever elastic forces that are the derivatives of their corresponding potentials. The figures from 1 to 8 on the right side of the poster represent the evolution of the total potential during the tip approaching, respectively the tip retracting from the surface.

Initially, the tip is far from the surface (fig. 1), the cantilever is not deflected, so the total potential has a minimal value, A, which is the tip state. When the tip approaches the surface (fig. 2) an horizontal displacement of the minimal value of the total potential can be observed. However, the tip remains in the position A, the first minimal value because no fluctuation can change its position. If the tip-surface distance still decreases (fig. 3), the tip position changes suddenly (fig. 4), the tip jumps in the minimum B, which correspond to the moment when the tip is in contact with the surface.

Continuing the tip approach, we enter in the repulsive domain. From the physical point of view, the tip cannot penetrate a surface infinitely rigid. The tip retracting starts when the tip-surface distance is minimal, the tip position corresponding to the point B in the potential representation (fig. 5). When the tip is pulled from the surface, the minimum B is moving horizontally (fig. 6, 7) in the Oz axis direction and another minimum, C, begins to appear. The tip state remains the B state until this minimum disappears, moment that corresponds to the tip-surface separation. It is the moment when the tip jumps in C position (fig. 8). For the numerical simulation of the approach-retract phenomenon, no kinetic energy was taken into account.

The movement of the symbolic tip in the figures at the bottom of the poster, right side, which is the movement of the white ball situated on the meshed surface, combined with color exchange of the potential line, bring to the user additional information concerning the approach-retract phenomena. The user became capable not only to feel the force intensity which is different at approach from the retract interaction, but also to see the moment of this two different actions.

Conclusions

In order to render the nano-world phenomena to the experimentalist in a haptic way as well as in a visual way, the physical and energetic analogy are presented and tested for the same approach-retract interaction. Using the representation in terms of potentials (Lennard Jones and elastic potentials), the experimentalist can distinguish not only the moments of tip approaching and retracting from the surface but also the differences between their characteristic parameters.

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