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Simulation of CAFM topography and current of structures based in high-k dielectrics and graphene

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Introduction

Nowadays, with the incorporation of new materials, as graphene or high-k dielectrics, in CMOS devices, their morphological and electrical characteristics must be deeply studied, since they could affect the device performance. As an example, the surface morphology of these materials could be a relevant variability source in ultrascaled devices [1, 2]. Conductive Atomic Force Microscopy (CAFM) has been shown to be a very powerful technique to study the topographic and electrical properties at the nanoscale [3, 4]. However, the CAFM characterization is affected by environment and/or experimental factors as the tip conductivity, radius, etc. In order to evaluate how each of the experimental parameters affects separately, new software has been developed. This tool allows to parameterize the CAFM experimental data measured on a given surface, generate topographical maps with the same physical characteristics, and evaluate the impact of such experimental factors. In this paper, three different structures have been simulated and compared with experimental data. Besides, the role of the tip geometry in each structure has been evaluated.

Methodology

To evaluate the usefulness of this new tool, three completely different structures have been measured with AFM and simulated with the software: polycrystalline HfO_2, graphene epitaxially grown on SiC, and amorphous HfO_2. For each structure, firstly, topographical AFM maps were measured and statistical characteristics such as roughness, grain size or grain boundary depth have obtained for a given temperature, tip radius or environment. Afterwards, through Monte Carlo (MC) simulation, the surface is generated using the acceptance-rejection method and the parameters (considered as inputs) obtained experimentally from the measured maps. Finally, the simulation inputs are optimized by least square method to obtain the best fit in the cumulative probability curves. For the simulations, the CAFM tip has been considered to be a semisphere [5], therefore the convolution algorithm is based on geometric considerations of the mutual excluded volume between tip and sample.

This tool can also simulate the current through gate dielectrics. From the band diagram, the quantum mechanical electron transmittance is calculated applying the Airy wavefunction approach [6]. This method is valid for any arbitrary band diagram. Finally, the current at each point of the generated map is calculated using the method in [7].

Results

Figure 1 shows three different experimental maps of (a) polycrystalline HfO_2, (b) graphene on SiC and (c) amorphous HfO_2 and their corresponding simulated images (e,d,f), respectively. The experimental images have been obtained with a nominal tip radius of 20 nm. We can observe that the simulated topography can reproduce the different analyzed samples. To quantitatively prove the good match between the experimental and simulated images, figure 2 shows the cumulative distributions of the heights for several simulations for each sample and the experimental image. Figure 3 shows the roughness value of the simulated images for different tip radius. Note that the rms dependence with the tip radius is greater when the surface geometry has structures of the same order of the tip size (polycrystalline structures). In the polycrystalline sample (with an average grain boundary width of 3.5 nm) the variation of the rms is 65% when the radius changes from 0 to 40 nm. However, in samples with

flatter surfaces this dependence is weaker: in the amorphous sample the variation is 9%.

In order to calculate the tunneling current through the gate dielectric Poisson equation is solved in order to obtain the potential barrier.

Figure 4 shows a schematic band diagram for a stack with two materials, where additionally the environment has been taken into account. Figure 5 shows a current map obtained for a polycrystalline HfO_2-Si structure. These simulations show that the current flows preferentially through the GB, as has been experimentally observed [4].

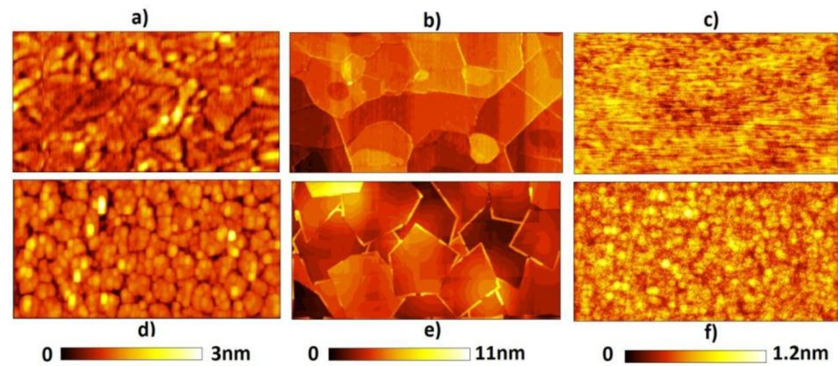

Figure 1. Experimental topography images a) HfO_2 polycrystalline (1x0.5 µm), b) graphene on SiC (4x2 µm) and c) HfO_2 amorphous (1x0.5 µm) and corresponding simulated images (e,f,g).

Conclusions

In this work, a simulation methodology, which allows to reproduce topography CAFM images of samples, has been presented. The generated maps have been compared with experimental results obtaining good agreement between them. Besides, current through a dielectric stack has been calculated from the band diagram at each point of the surface. The current calculation considers the morphology and the electrical properties of the analyzed stack, the environment and CAFM tip properties. This simulation method can be very useful for the evaluation of the unavoidable experimental effects intrinsic to the CAFM technique. Also, the tool can be used to generate high amount of data, reducing the number of long time consuming CAFM measurements.

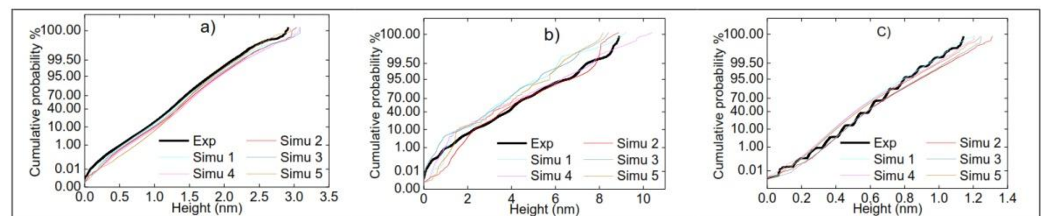

Figure 2 Height cumulative probability of experimental and several simulated maps for each sample. a) HfO_2 polycrystalline, b) graphene on SiC, c) HfO_2 amorphous.

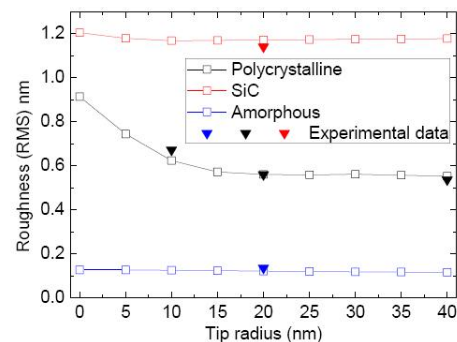

Figure 3 Roughness as a function of the tip radius. The empty symbols represent simulation points and the filled symbols are experimental measurements.

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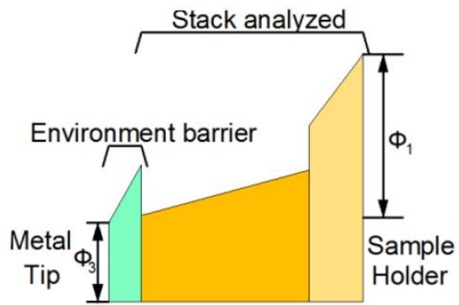

Figure 4 Schematic band diagram showing any stack with two different materials and having into account the environment barrier.

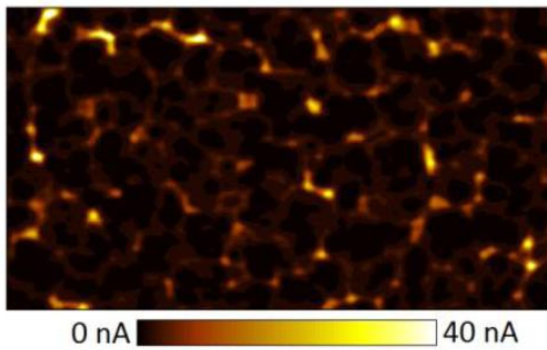

Figure 5 Simulated current image corresponding to the topography map in fig.1d. The applied bias is 2 V.