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VisualTAPAS: an example of density functional theory assisted understanding and simulation of anisotropic etching

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Abstract

VisualTAPAS is a self-contained, user-friendly, graphical user interface based simulator of wet etching and deep reactive ion etching with multi-masking capabilities, built upon an octree representation of the silicon substrate (www.fyslab.hut.fi/~mag/VisualTAPAS/Home.html). The program allows the use of a wide range of kinetic Monte Carlo (KMC) and cellular automata time-evolution algorithms, including a fast octree search algorithm for the KMC simulations. 'VisualTAPAS' stands for 'visual three-dimensional anisotropic processing at all scales'. The use of the term 'visual' stresses the interactive visual capabilities of the program.

Here, a brief history of the evolution of VisualTAPAS as a research tool will be presented: from the initial efforts, explaining the anisotropy of wet etching as a result of steric hindrance using a combination of density functional theory (DFT) and KMC simulations, to the most recent implementation, focusing on the propagation of the etch front for engineering applications by making use of the analytical solution of the continuous cellular automaton (CCA) method; and in between, a recent example of DFT assisted understanding of the effects of metal impurities on the surface morphology of the etched surfaces will be presented.

We try to bridge together three complementary simulation tools, namely, DFT, KMC and CCA methods. Our experience with the use of the three methods for the simulation of anisotropic etching shows that DFT is very useful and, many times, an unavoidable approach. Similarly, the KMC approach is the method of choice for understanding the large variety of etched surface morphologies while the CCA is an outstanding tool for the simulation of the process at an engineering level.

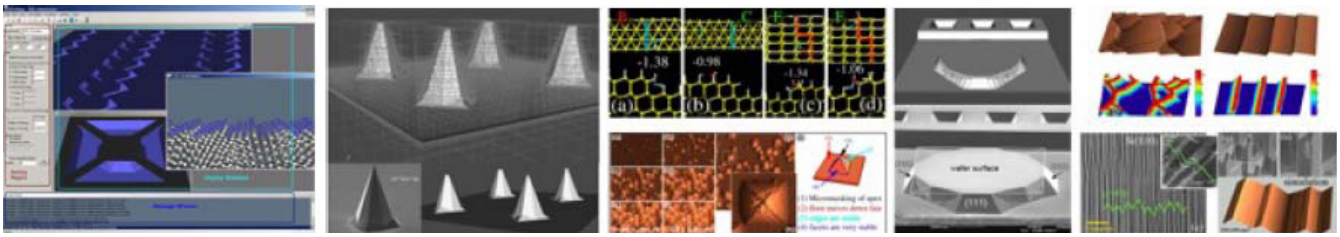

Figure 1. Graphical user interface and examples of simulations using VisualTAPAS.
(This figure is in colour only in the electronic version)

