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Understanding the hillock-and-valley pattern formation after etching in steady state

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Abstract

We derived a simple mean field model that accounts for the formation of hillock-and-valley patterns after etching in steady state. The mechanisms and their interrelations that lead to these patterns experimentally observed are described. Hillocks and valleys present characteristic size distributions that are governed by the relative etching rates of particles in different sites. In particular, we focus on how etching processes determine the surface morphology and the resulting hillock size distribution. The dependence of these mechanisms on the model parameters is specifically addressed. Monte Carlo simulations were carried out in one dimension using a restricted-solid-on-solid model with nearest neighbor interactions. The outcomes of the mean field model and Monte Carlo simulations are compared.

Keywords: Monte Carlo simulations; Etching; Surface structure, morphology, roughness and topography

1. Introduction

Anisotropic wet chemical etching remains the most widely used processing technique in silicon micromachining. Much effort has been dedicated to the characterization and understanding of the surface morphology since micromechanical devices continuously reduce in size and their performance requires a very smooth surface. For Si surfaces, highly anisotropic dissolution ratios are well known, with (1 0 0) and (1 1 0) dissolving much more rapidly than (1 1 1), as reported for etchants such as KOH and NH_4F [1–17]. In these investigations the most frequent surface inhomogeneities reported are the pyramidal etch hillocks.

The production of a smooth surface is easily visualized within a site-dependent interaction picture. In a first analysis, we expect more coordinated atoms to be etched with a slower rate than those having fewer neighbors. Thus, any type of protuberance or pit would be unstable and should tend to disappear leading to a smooth surface. For a protuberance or a pit to form, a low or high etching rate region must be present. Etching rates can be different close to a crystal defect, such as a dislocation. Also, an external agent, such as an adsorbed contaminant or a reaction product, can reduce etching and thus a hillock might form.

Etching of vicinal Si(1 1 1) occurs by the continuous retreat of the steps. In this case, the surface morphology is dominated by step roughening since terraces are rarely attacked. It is found that $[\bar{1}\,\bar{1}\,2]$ step sites are etched much faster than $[1\,1\,\bar{2}]$ step sites. When Si(1 1 1) miscut in the $[\bar{1}\,\bar{1}\,2]$ direction is etched a characteristic morphology appears. The etched step presents many straight step segments oriented in the $[1\,1\,\bar{2}]$ directions that constitute two-dimensional etch hillocks giving a shark's tooth shape to the structure [18]. Interestingly, some authors attributed the appearance of these two-dimensional hillocks to some type of micromasking [9–13].

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Instead of resorting to an external origin for the apices stability, Hines and co-workers took into account factors such as steric hindrance and lattice strain that can play a role in relative site reactivities [18–20]. They proposed that the topmost site of a two-dimensional hillock is unhindered, unstrained, and then relatively resistant to etching. This means that etching rates are only site specific. Thus, the resulting patterns are only the consequence of particle removal; other mechanisms, such as diffusion, are not allowed. This has been considered to have a minor role in the formation of hillocks [17,21–23].

We are especially interested in the general aspects of the etching processes and resulting morphology. The main goal of using a simple one-dimensional model is to explain the experimentally observed step morphology in a framework in which only two parameters control the resulting surface pattern. Other authors have made more realistic and detailed models taking into account the crystal structure and the bonding energetics. However, the complexity and the large number of parameters involved in these models make very difficult to determine the basic mechanisms responsible for the resulting surface morphology. With our model we reproduced the pyramid-and-valley patterns that regularly appear under steady-state etching in Si(1 0 0) [24].

Extending previous work [24–26], we explore and describe, within a site-dependent detachment probability framework, the mechanisms responsible for hillock formation and their interrelation that contribute on the final surface morphology. We analyze in detail the underlying dynamics that lead to non-trivial hillock-and-valley patterns using a restricted solid-on-solid one-dimensional substrate model for Monte Carlo simulations. We focus on the mechanisms involved in the formation of hillocks and how the surface maintains a specific morphology under steady state. We develop a simple mean field model that includes the relevant site dependent mechanisms in order to explain the experimentally observed patterns. Finally, we compare the model predictions with the outcomes of Monte Carlo simulations.

2. Monte Carlo simulation

We represent the step with a one-dimensional vector where each element accounts for the height at the surface site. In the simulations, particles can be removed (etched) from the step according to its site-specific etching rate. To accomplish this, sites were visited at random and their neighborhoods were inspected to determine the detachment probability of the surface particle. In our model, only first neighbor interactions were considered and particle rearrangement was not allowed (there was no diffusion). The parameters that determined the step morphology were the removal rates of three distinct sites related to the particle coordination number. Particles available to be removed could have two (step site), one (kink), or zero (point site or apex) first neighbors along the step with etching rates k_i, where i is the coordination number.

Our simulation was based on the restricted solid-on-solid (RSOS) model in which there were no overhangs and a maximum height difference of one between neighboring columns was allowed [27]. Thus, the substrate configuration was completely determined by the heights of each column relative to the flat reference surface. The evolution of the system configuration was found using the standard Monte Carlo method for a one-dimensional array of 1000 sites. Periodic boundary conditions were used to avoid edge effects. The system evolved with successive annihilations of substrate particles until it approached a steady-state configuration. We checked that steady state was reached by monitoring the surface roughness evolution.

The geometry we are using leads to a model that is very similar to that used in [18–20]. That is why we obtained almost the same results than those found in these references. Specifically, the main relevant parameters used by Hines and co-authors are the same parameters we used.

3. Basic etching mechanisms

After performing Monte Carlo simulations for a variety of site-specific rate constants, it is found that slow-etching step sites and relatively stable hillock apices are needed for hillocks to form [18–20,24]. Thus, kinks must be the fastest etching sites, and a value of 1 was adopted for their detachment probability. Step sites must be robust, and we explored different values for the detachment probability from them; the results presented here correspond to a probability of 0.005.

As expected, etch hillocks developed for relatively small values of k_0. The transition from a flat surface to a hillocked one takes place in a small range of the apex etching rate. Fig. 1 shows the morphology dependence on k_0. Interestingly, hillock-and-valley patterns are only stable for a limited range of the apex etching rates (we mean by a valley as a flat region between hillocks). This morphology, in which hillocks form and co-exist scattered on a surface of limited roughness, is regularly observed in silicon etching. We are specifically interested in the mechanisms responsible not only for the hillock formation but also to explain what determines their size.

Monte Carlo results show that steps present hillocks of very different sizes. At first glance, it seems that hillocks can adopt any size at random. However, we found that the hillock size distribution presents an exponential distribution when valleys are also present [25,26]. The surface temporal evolution demonstrates that small hillocks are continuously formed and annihilated. Conversely, large hillocks seem to propagate while their apices perform a random walk parallel to the step edge. After enough time, however, large hillocks can shrink and eventually disappear.

Next, the different mechanisms present during the step evolution as it is etched will be analyzed and a mean field model will be introduced.