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THEORY OF WEAR: FROM THE ABRASION TO THE SELF-ASSEMBLY

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Abstract: In a scratching AFM experiment, the continuous passage of a sharp tip produces a flux of adatoms stripped off by their initial locations. Such flux has as secondary effect the formation of self-assembling processes such as ordered small atomic clusters, dots or larger corse-grained mounds. In this paper, we suggest a continuum approach based theory that should capture the basic mechanisms producing the formation of such structures. The accurate knowledge of such self-assembled structures is important for two main reasons. First one, looking at the self-assembled structures it should be possible to have an indirect measure of the incidence of the wear basic mechanims involved during the AFM scratching test. Second one, the patterned structures produced could be used as a base for eventually mature growth processes.

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1. Introduction

On nanoscale, in many devices the surfaces and their properties play a major role respect to bulk properties. During the contact of two surfaces in relative

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motion, dissipative forces and damaging can limit the performances of the devices on nanometer technology. As a consequence, in the last two decades, many knowledge has been addressed to deal out the tribological properties at the atomic and molecular scale, [1]. In the last years, some experiments had proposed meaningful occurrence for the abrasive wear mechanims, [6], [9], [2], [8], [5], [10]. In such experiments, the wear process is as follows: a probe tip scans repeatedly a small area of the surface of interest. The stressing passage of the tip produce a removed debris (adatoms). In some cases, looking at larger areas centered around the worn small area, it is possible image surface structures such as atomic clusters, or larger aggregates. The basic wear mechanims involved are rather complicated, and their theoretical mature understanding is largely uncomplete. In this paper, we propose a possible new approach for the comprehension of some wear mechanims looking at the surface growth patterns induced by the abrasive wearing AFM scratching tests. The idea underlying our theory is the following: the structures formed by the adatoms stripped off by the AFM tip are an indirect measure of the basic wear mechanisms, the adatoms are the debris produced and their ability to re-organize ordered structures is strongly dependent by their rate production.

2. The Model for Wear Production and Growth Surface Processes

The growth of regular patterns as derived by an AFM induced wear process can be described by a continuous height function $h(x, y, t)$, where x,y are the surface coordinates. On the average, the surface receives a flux of adatoms, F. This flux depends by the quality of the wear activated production of adatoms, for sake of simplicity, the adatoms have the same volume Ω, which corresponds to the mean volume of the debris. In reality, during the scratching, the stripping off of atomic clusters from the worn surfaces should be taken in consideration. The various processes by which matter is redistributed along the surface are represented by some functions of the derivatives of h with respect to space coordinates. Moreover, if the whole stripped off mass goes in the growth process, then a mass-conservation condition would be fulfilled:

$$\partial h/\partial t = \Omega \nabla \cdot J = F \,, \tag{1}$$

where J is the adatom (debris) number current density within the surface. The equation (1) connects the time dependent growth process to the wear production of the debris adatoms. In fact, in our case, the current density is referred to the surface diffusion current of adatoms produced during the stressing passage

of the AFM probe tip. The probability that an atom is stripped off during the passage of a probe tip is given by:

$$\Gamma = \nu \exp -[E_b - \delta E_s]/k_B T \,, \tag{2}$$

where E_b is the binding energy, δE_s represents the stress-induced deviation induced by the AFM tip contact, k_B is the Boltzmann's constant and T is the temperature. The stress-induced deviation is a combined effect of the compression and shear stresses during the passage of the probe tip and it lowers the energy barrier making possible the stripping off of the atoms from the primitive positions. After the stripping off, the debris diffusively moves along the surface. The surface diffusion motion of the debris is then a function of the surface landscapes energy. The landscape energy is the principal responsible for the possible self-assembly structures borning by the interaction of the debris continuously produced during the scratching process.

The total number density of adatoms produced by the wear abrasion process and freely available for the growth surface processes and subsequent patterning is given by for unity of time [3]:

$$F = n\Gamma \,, \tag{3}$$

where F represents the number of the adatoms produced during the wear process, n is the total surface atom density, and Γ is given by the equation (2). The rate production of F is crucial for the nucleation of clusters and subsequent growth of regular structures. For the rate production of F we propose two possible functional form. The first one provides a sigma functional dependence by the Γ rate because the wear debris production can follows a nucleating process, [3]. On contrary, another suitable choice for the rate dependence could be a shot-noise like function. In the next section, we will integrate a simple two-equations time evolution cluster density systems making use of the two rate debris production.

3. Surface Growth Induced by Wear Mechanisms

In this section, we give an evaluation of the number density of the clusters making use of the mean-field approximation. It is possible to consider a time evolution density quantification for atomic clusters aggregation with time dependent rates. The time dependent equations for the density of the clusters N is:

$$\dot{N}_1(t) = F(t) - DNN_1(2N_1 + N) \,, \tag{4}$$

$$\dot{N}(t) = D(N + N_1)N_1^2(t)\,, \tag{5}$$

where N_1 represents the single adatom cluster density. The rate flux of adatoms, $F(t)$, depends by the wear basic mechanisms. In this sense, the formation of clusters is an indirect measure of the fundamental wear activation mechanisms. On possible form for the rate flux, $F_1(t)$, is a shot noise-like form as:

$$F_1(t) = \eta \sum_{k=0}^{\infty} \delta(t - T)\,, \tag{6}$$

where η denotes the numerical density of adatoms produced during the AFM scratching and T is the period time between two subsequent adatoms produced during the stressing probe tip passage. Analogously, it is possible to have a continuous rate flux given by the nucleation of wear domains during the progressive AFM scratching, [3]:

$$F_2(t) = \eta(1 - \exp(-\alpha t)) \tag{7}$$

where α is a parameter which depends by the rate of nucleation. The rate flux as expressed by equation (7) denotes a sigma function for the progressive production of adatoms during the AFM scratching.

A simple evolution equation that captures much of the relevant physics can be derived in the limit of a perfectly rigid substrate and in a small slope approximation near the Asaro-Tiller-Grinfeld instablity threshold. The shape of such growth film surface evolves due to the surface diffusion to decrease the elastic energy of the substrate as follows [7]:

$$\partial_t h = -\nu_w + D\sqrt{1+ \mid \nabla h \mid^2}\nabla_s^2[\epsilon(h) + \Phi]\,, \tag{8}$$

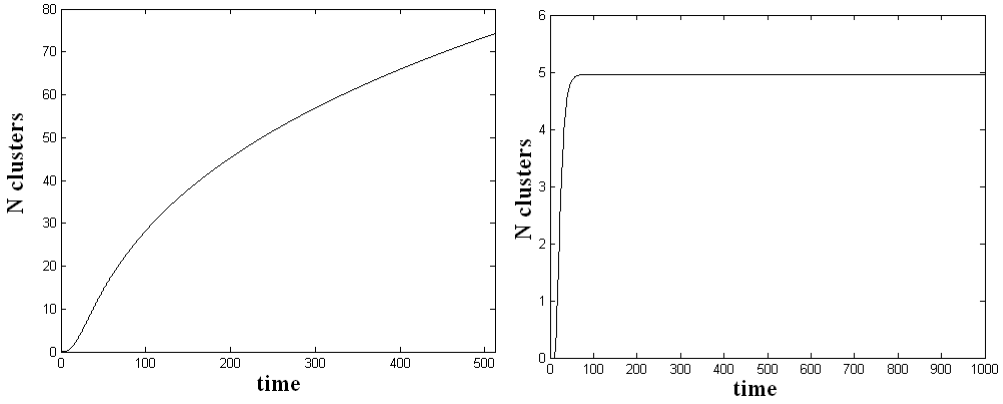
where D is a constant proportional to the surface diffusivity, ϵ is the elastic energy density at the surface, Φ is a wetting chemical potential, [7]. The surface chemical potential is the variation of the total free energy calculated starting from the rigid substrate:

$$\mu = \epsilon(h) + \Phi = \delta E/\delta h = \delta(E_{el} + E_{surf})/\delta h\,, \tag{9}$$

where E_{el} is the total elastic energy (we use the state of the planar surface as the reference state for the energy), E_{surf} is the surface energy, and $\delta E/\delta h$ is the functional derivative of the total free energy E. The surface free energy is connected to the surface height via the expression:

$$E = E_{el} + E_{surf} = E_{el} + \int \gamma\sqrt{1 + (\nabla h)^2 ds}\,, \tag{10}$$

where γ is the surface tension. A growth process as described by equation (10) shows that there is a critical film thickness h_c below which the film is stable. For larger film thickness there is a long range of instability. It is possible to manage



(a) (b)

Figure 1: Figure 1 shows the two possible regimes occurring depending by the flux-type produced during the wear abrasion process. The adatom flux generated by nucleating worn islands gives a sigma-like curve describing the time evolution of the multiple dots self-assembling, Figure 1(a). On contrary, the shot-noise like flux generates a suddenly saturating curve involving the production of few islands. Such islands undergo to a corse-graining process giving the typical mounds observed experimentally by Gnecco et al [6]. The two regimes captured by the mean-field nucleations equations implies that the growth surface regime depends by the nature of the flux and ultimately, by the nature of the wear activated mechanisms.

equation (10) in order to simplify it and to draw a numerical quantification. To this end, we need to introduce a lenght scale L characterizing the thickness of the film ($L = h_c$) and assume that the lenght scale for the variations in the lateral directions is much larger. Analogously, introducing a suitable coiche for the time scale, we can obtain the following equation written in the new rescaled variables [7], [4]:

$$\partial_t h = -\nu(x,y) + \nabla^4 h + \beta\nabla^6 h + \nabla^2[h\nabla^2 h + 0.5 \mid \nabla h \mid^2], \qquad (11)$$

where $\nu(x,y)$ is the local abrasion rate. The equation (11) can be solved numerically. Details are included in [4], here, we can comment that for a suitable choice of the parameter used for the numerical solution of equation (11) the corse-grained regime (mounds) is absent, and only the cluster regime (dots) is captured, as experimentally observed by [9].

4. Conclusions

Wear basic mechanims are still unknown. Scratching AFM experiments, where the continuous passage of a sharp tip produces a flux of adatoms stripped off by their initial locations, are opening new possibilities for a comprehension of such basic mechanims. A secondary effect of a scratching experiment is the formation of self-assembling processes such as ordered small clusters, dots or larger corse-grained moulds. Looking at the self-assembled structures is possible to have an indirect measure of the incidence of the wear basic mechanims involved during the AFM scratching test. In turn, the patterned structures produced could be used as a base for mature growth processes. In this paper, a continuum approach based theory that should capture the basic mechanisms producing the formation of such structures has been preliminarily presented.

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