Numerical study of the thermal relaxation of self-affine surfaces

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Complex self-affine surfaces can be obtained through various natural and technological processes. They exhibit fractal structure which develops dynamically during growth. Formation of these non-equilibrium morphological systems has been extensively studied [1]. However the relaxation of their shape after the growth is much less investigated, though controlled flattening of rough surface is important issue in many applications. In fact, the relaxation dynamics of complex systems can be quite complicated, and the search for dynamics scaling and universality is recent. Such approach is useful for proper description and characterization of surfaces, but has implications too.

In this presentation [2], we study disappearance of the self-affine roughness of surfaces by thermal atomic rearrangement. We use Monte-Carlo numerical simulations to model the flattening process. In thermal shape relaxation, three main mass transport mechanisms may be involved: 1) evaporation-condensation mechanism where atoms leave the surface and move onto the substrate to recondensate somewhere else; 2) surface self-diffusion process where only surface atoms migrate along the surface leading to smoother structures; 3) viscous flow for which volume atoms are also mobile. Here, the mechanism 3) is not considered (we deal with the low values of the heating temperature).

Various self-affine solid surfaces are generated by random ballistic deposition model of monodisperse particles of radius a, or by the Eden model [3]. Transport is performed following essentially the algorithm of Irisawa et al [4]. The rate of diffusion along the surface is $\exp(-mE_b/kT - nE_d/kT)$, where m is the number of bonds to be broken when atom moves and E_b is the bond energy. E_d is the barrier energy per bond and n is the number of neighboring bonds for an atom which diffuses along the surface. The rate of evaporation of an atom from the surface to become an adatom which moves randomly on the surface is $\exp(-rE_b/kT - \Delta\mu/kT)$, where r is the number of bonds that break when atom leaves the surface and $\Delta\mu$ is the chemical potential involved in the growth process.

As the thermal process acts, the Hurst exponent – which characterizes the fractal roughness –, decreases. It is consequence of progressive disappearance of the short wavelength fluctuations of the surface. This behavior may be seen through horizontal cuts of the surface close to it. Particularly significant is the cut at height equal to the one if the surface were completely flat. From a very complicated initial pattern, the mass distribution transforms into a set of islands. The islands of smallest diameter then disappear or merge into larger ones. At a given time, the pattern of islands crosses the percolation threshold, then the self-affine scaling disappears completely.

References

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