NANO-PATTERNING OF SURFACES BY ION SPUTTERING: NUMERICAL STUDY OF AN ANISOTROPIC KURAMOTO-SIVASHINSKY EQUATION

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1 Introduction

Ion beam sputtering is one important technology which operates in nonequilibirum conditions and allows the processing of materials and structures outside the limits of the equilibrium thermo-dynamics. The theoretical comprehension of such process is still an ongoing challenge and their mathematical modeling needs more development. Our effort aims toward the implementation of a numerical scheme to solve a model proposed to the ion beam sputtering erosion.

The phenomenon consists on the ionic bombardment of a surface, spontaneously developing a well-ordered periodicity over a large area under certain conditions. This physical process responsible for the formation of periodic structures on the previously surface is called sputtering. Depending on the energy of the incident ion, a train of collision event may be established, resulting in the ejection of atoms from the matrix. The morphology of the surface can drastically change due to these sputtered atoms, being responsible for the appearance of unexpectedly organized patterns, such as ripples and hexagonal arrays of nanoholes.

The Kuramoto-Sivashinsky equation is deterministic and highly nonlinear, being capable of producing a great variety of morphologies, making it a strong candidate to represent the complex structure formation on sputtered surfaces. In the present endeavor, a finite-difference semi-implicit splitting scheme of second order in time and space is proposed to numerically solve an anisotropic Kuramoto-Sivashinsky equation subjected to periodical boundary conditions for two dimensional surfaces.

2 Numerical scheme

One of the simplified and dimensionless form of the anisotropic Kuramoto-Sivashinsky reads:

$$\begin{aligned}\frac{\partial \bar{h}}{\partial \tau} &= -\bar{\alpha}\bar{h} + \bar{\mu}\frac{\partial^2 \bar{h}}{\partial X^2} - c^2\frac{\partial^2 \bar{h}}{\partial Y^2} + \bar{\nu}_x\left(\frac{\partial \bar{h}}{\partial X}\right)^2 - c^3\left(\frac{\partial \bar{h}}{\partial Y}\right)^2 \\ &\quad -D_{XX}\frac{\partial^4 \bar{h}}{\partial X^4} + D_{XY}\frac{\partial^4 \bar{h}}{\partial X^2 \partial Y^2} + c^2\frac{\partial^4 \bar{h}}{\partial Y^4} \\ &\quad -\bar{K}\left(\frac{\partial^4 \bar{h}}{\partial X^4} + 2\frac{\partial^4 \bar{h}}{\partial X^2 Y^2} + \frac{\partial^4 \bar{h}}{\partial Y^4}\right) \end{aligned} \quad (1)$$

where $\bar{h}$ and τ are, respectively, the surface height function of the external atom layer and the time dependency of the transient model, with X and Y as the domain space coordinates. The function c represents the cosine of the incident angle θ. Equation. 1 presents a damping term $-\alpha\bar{h}$, with α being damping coefficient, contributing to the smoothening of the surface. Finally, K takes into account the surface diffusion effects, which varies with temperature. The parameters μ, ν_x, D_{XX} and D_{XY} are anisotropy coefficients and also function of θ.

We propose the following second order in time Cranck-Nicolson semi-implicit scheme for solving Equation 1 with $a_\mu = 4$, high temperatures and $< 65.3°$ [1]:

$$\frac{\bar{h}^{n+1} - \bar{h}^n}{\Delta\tau} = \Lambda_X\frac{\bar{h}^{n+1} + \bar{h}^n}{2} + \Lambda_Y\frac{\bar{h}^{n+1} + \bar{h}^n}{2} + f^{n+1/2}$$

Since the operators $\Lambda_X^{n+1/2}$, $\Lambda_Y^{n+1/2}$ and the function $f^{n+1/2}$ contain terms in the new stage we do internal iterations at each time step according to:

$$\begin{aligned}\frac{\bar{h}^{n,m+1} - \bar{h}^n}{\Delta\tau} &= \Lambda_X\left(\bar{h}^{n,m+1} + \bar{h}^n\right) \\ &\quad +\Lambda_Y\left(\bar{h}^{n,m+1} + \bar{h}^n\right) + f^{n+1/2}\end{aligned}$$

The splitting is made according to the Douglas second scheme [2]

$$\begin{aligned}\frac{\tilde{\bar{h}} - \bar{h}^n}{\Delta\tau} &= \Lambda_X\,\tilde{\bar{h}} + \Lambda_Y\,\bar{h}^n + f^{n+1/2} + (\Lambda_X + \Lambda_Y)\,\bar{h}^n \\ \frac{\bar{h}^{n,m+1} - \tilde{\bar{h}}}{\Delta\tau} &= \Lambda_Y\left(\bar{h}^{n,m+1} - \bar{h}^n\right)\end{aligned}$$

3 Results and Discussion

3.1 Initial Pattern: Random Structure

The first case analyzed was for a mesh with 256 × 256 points with a randomly generated initial pattern, ranging from 0 to 0.1. Since the linear stability analysis reveals a value of $\lambda_c = 18$ for the critical wavelength corresponding to the maximum growth rate in the $\vec{1}_x$ direction, each wavelength of the final pattern was expected to be represented by approximately 9 points.

Figure 1 shows the steady state hexagonal structure clear of defects, after the emergence of hexagonal modes from the initial random pattern. The Fast Fourier Transform (FFT) is also displayed for the central part of the domain (Figure 2).

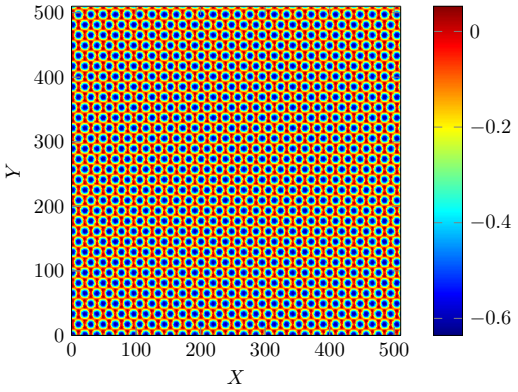

Figure 1: $\bar{h}_n$ Top XY view for $\tau = 49, 200$

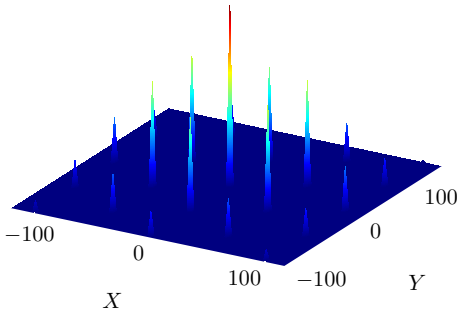

Figure 2: $\bar{h}_n$ Fourier Transform for $\tau = 49, 200$

3.2 Initial Pattern: Monomode $\vec{q} = q_o\vec{1}_x$

Another case of interest studied was for an initial pattern with sine function in the X direction, which represents a monomode 1D structure with wavevector $\vec{q} = q_o\vec{1}_x$. The pattern started with 14 wavelengths, being approximately half of the total number of wavelengths in the steady state from the previous case, which agrees with the critical wavelength calculated from the linear stability analysis and is placed inside the stable domain. Figure 3 displays the final state obtained, which is a 1D structure with 27 wavelengths, and Figure 4 shows its Fourier Transform. The wave amplitude goes initially from (0;0.1) to (-0.4;0) in the final state, which is also consistent with the physical phenomenon of surface erosion. Although it seems that the steady state was reached, hexagonal modes are expected to grow after more time steps.

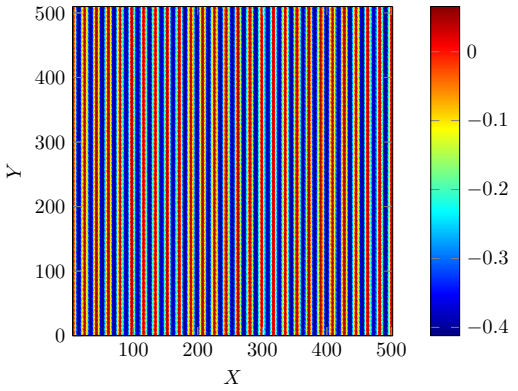

Figure 3: $\bar{h}_n$ Top XY view for $\tau = 150$

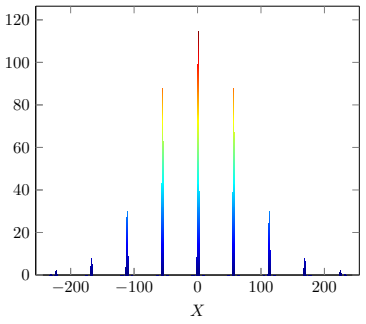

Figure 4: $\bar{h}_n$ Fourier Transform for $\tau = 150$

4 Conclusions

In the present paper we have developed a finite-difference time splitting scheme for solving an anisotropic Kuramoto-Sivashinsky equation to describe a surface eroded by ion bombardment. Hexagonal patterns grew from a domain with random initial conditions, and for the monomode $\vec{q} = q_o\vec{1}_x$ case the wavelength split in two, meeting the critical wavenumber from the linear stability analysis. Both simulations were physically consistent with the sputtering phenomenon, reproducing ripple and hexagonal structure formation dynamics.

5 Acknowledgments

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References

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