Nano-patterning of surfaces by ion sputtering: Numerical study of the Kuramoto-Sivashinsky Equation

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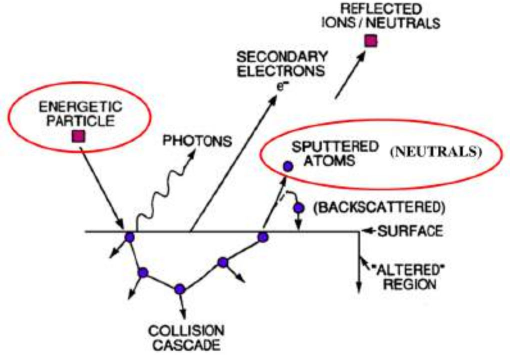
Overview

Sputtering

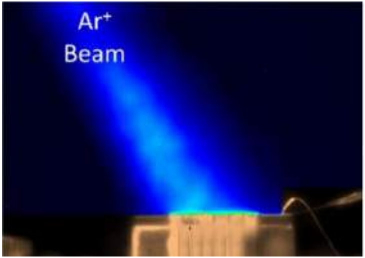
- Physics of Sputtering

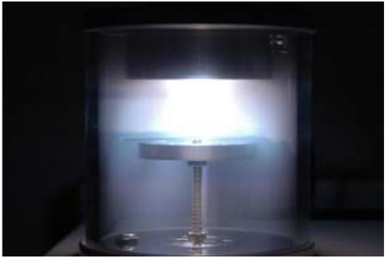


- Applications: thin film deposition, micromachining, pattern etching for the fabrication of integrated circuits and chemical analysis

Sputtering

- Ion Beam x Glow Discharge Sputtering





- Sputtering yields:
  - $E < 1KeV : S = \dfrac{3\alpha}{\pi^2} \dfrac{M_1 M_2}{(M_1 + M_2)^2} \dfrac{E_i}{E_L}$
  - $E > 1KeV : S \sim (Z_1 Z_2) \dfrac{M_1}{M_1 + M_2} S_n(E)$

Experimental results

- Two main classes of surface morphology by ion sputtering according to experimental results:
  - Periodic ripples on the surface
  - Rough eroded surfaces
- Experimental data and parameters:

i) Ripple formation

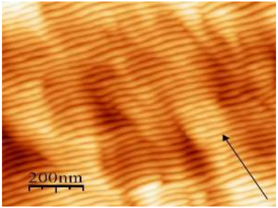
- Angle of incidence
- Temperature dependence
- Ion energy
- System chemistry

ii) Kinetic roughening

- Temperature dependece
- Ion energy

Experimental results

Rippled patterns formed by ion sputtering have close relatives in nature:



(a) Ar^+ sputtering on Si

(b) Namib desert

(c) Cloudy sky

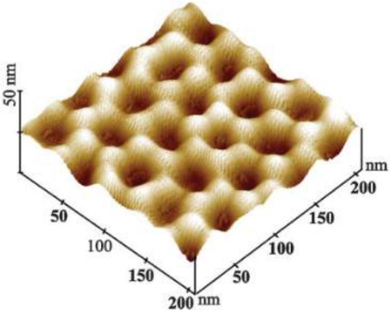
(d) Ripples on the water

Experimental results

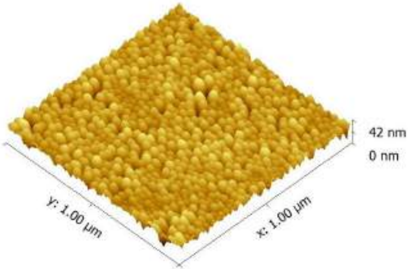
- Bradley and Harper theory (HP): theoretical approach describing the process of ripple formation on amorphous substrates
  - Ripples are a result of a surface instability caused by the curvature dependence of the sputter yield.
  - Wavelength and orientation prediction in agreement with numerous experimental results
  - Cannot account for surface roughening
- A nonlinear theory is required to model the time evolution of ion-sputtered surfaces and predict their morphology:
  - Short time scales: describe the development of a periodic ripple structure
  - Large time scales: the predicted surface morphology should be rough or dominated by new ripples

Experimental results

Experimental data and imaging (AFM):



3D image of hexagonally ordered nanoholes on a Ge surface (Ga^+ FIB bomdardment) obtained from AFM data



AFM image of a nanodot pattern created by Ar^+ sputtering on GaSb(001)

Theoretical approaches

Kardar-Parisi-Zhang equation (KPZ):

$$\partial_t h = \nu \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta$$

- Nonlinear stochastic partial differential equation
- Describe the time evolution of a nonequilibrium interface
- $\eta\,(\vec{x}, t)$: noise, reflects the random fluctuations in the process
- EW equation, $\lambda = 0$: equilibrium fluctuations of an interface which tries to minimize its area under the influence of external noise
- Scaling properties may change drastically due to anisotropy (AKPZ)

Theoretical approaches

Kuramoto-Sivashinsky equation (KS):

$$\partial_t h = -|\nu|\nabla^2 h - K\nabla^4 h + \frac{\lambda}{2}(\nabla h)^2$$

- Deterministic equation, originally proposed to describe chemical waves and flame fronts
- Chaotic solution rises from its unstable and highly nonlinear character
- 1D: for long time and length scales, the surface described by the KS equation is similar to the one described by the KPZ equation; for short time scale solution, the morphology is reminiscent of ripples
- 2D: contradictory computer simulations

Numerical scheme

Governing equation:

- An anisotropic damped Kuramoto-Sivashinsky equation was adopted for the present study
- One simplified dimensionless form of such equation can be described as follows:

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

Numerical scheme

Semi-implicit scheme:

- We propose the following second order in time Cranck-Nicolson semi-implicit scheme for solving the target equation with $a_\mu = 4$, high temperatures and $\theta < 65.3^\circ$:

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

- Including the factor $1/2$ into the operators Λ_X and Λ_Y , they may be defined as follows:

$$\Lambda_X = \frac{1}{2}\left[-\frac{\bar{\alpha}}{2} - (D_{XX} + K)\frac{\partial^4}{\partial X^4}\right]$$

$$\Lambda_Y = \frac{1}{2}\left[-\frac{\bar{\alpha}}{2} - K\frac{\partial^4}{\partial Y^4}\right]$$

Numerical scheme

Internal iterations:

- 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:

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

where the superscript $(n, m+1)$ identifies the "new" iteration. The iterations proceed until the following criteria is satisfied:

$$\frac{max\,|\bar{h}^{n,m+1} - \bar{h}^{n,m}|}{max\,|\bar{h}^{n,m+1}|} < \delta$$

Numerical scheme

The splitting scheme:

- The splitting of the target equation is made according to the Douglas second scheme (also known as "scheme of stabilizing correction"). It is designed as follows:

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

Linear stability analysis

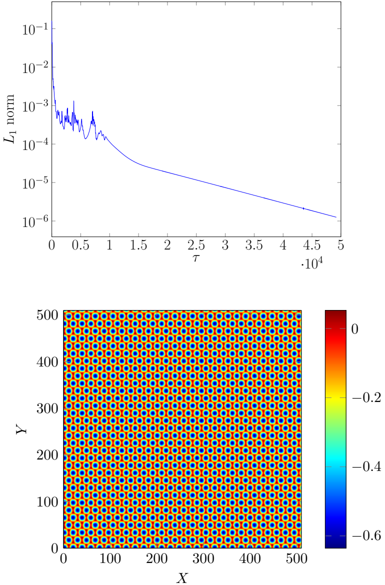
- In Fourier transform, for small perturbations, the governing equation may be written as:

$$
\begin{aligned}
\bar{h}_p(\vec{q}) &= \bar{h}_o e^{i(q_x X + q_y Y)} e^{\sigma_\tau} \\
\sigma_\tau \bar{h}_p(\vec{q}) &= \big[-\bar{\alpha} + (-\bar{\mu} q_x^2) + (-\bar{\nu} q_y^2) - D_{XX} q_x^4 + D_{XY} q_x^2 q_y^2 \\
&\quad + D_{YY} q_y^4 - \bar{K}(q_x^2 + q_y^2)^2 \big] \bar{h}_p(\vec{q})
\end{aligned}
$$

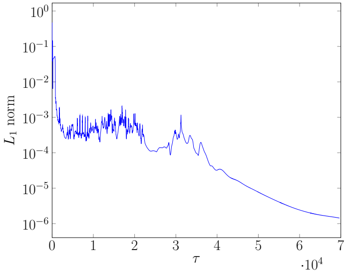
- The anisotropic coefficients D_{XX}, D_{XY} and D_{YY} can be hidden for an easier manipulation of the equation. Besides, we may consider $q^2 = q_x^2 + q_y^2$.

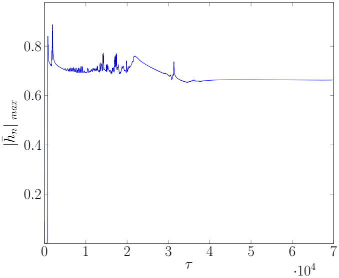
$$
\sigma_\tau = \epsilon - \bar{K}(q^2 - q_c^2)^2 - (|\bar{\mu}| - |\bar{\nu}|) q_y^2
$$

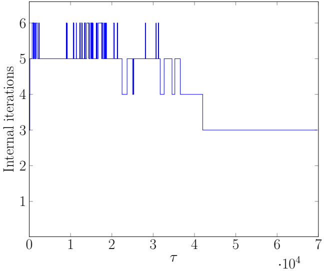
Random initial case

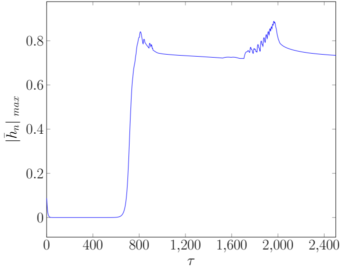


Initial pattern: monomode $q_o\vec{1}_x$

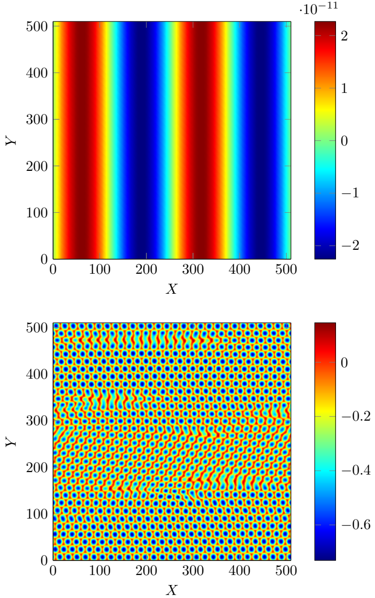




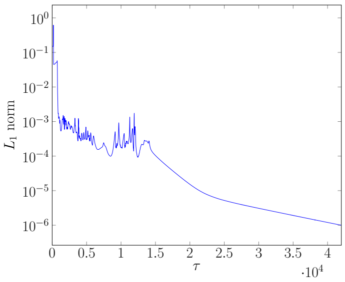


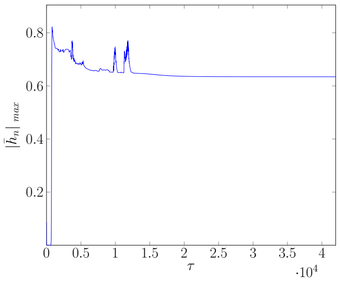


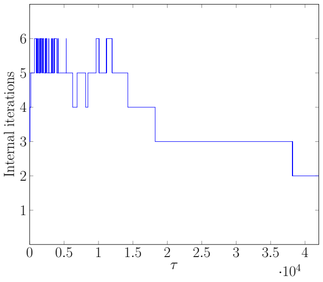
Initial pattern: monomode $q_o\vec{1}_x$



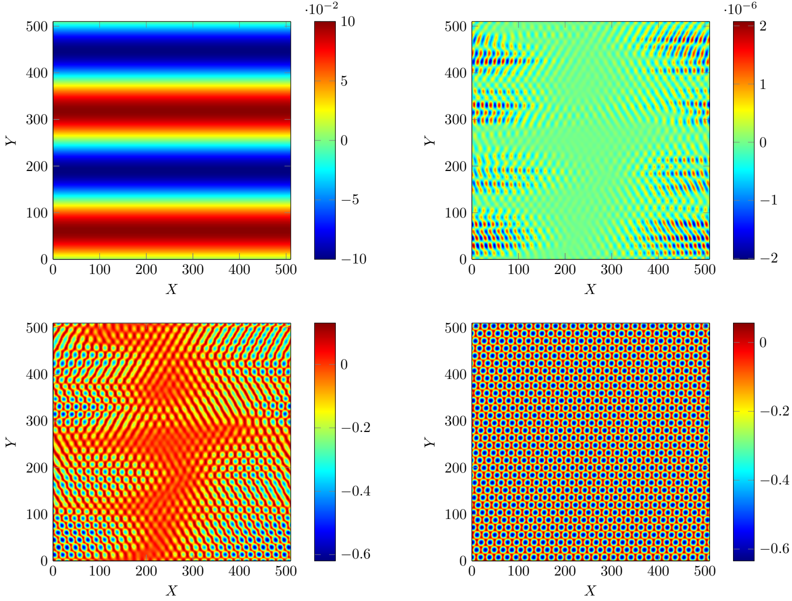
Initial pattern: monomode $q_o\vec{1}_y$







Initial pattern: monomode $q_o\vec{1}_y$



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