Langevin approach for plasma-surface interaction: turbulent sputtering and surface morphology

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Introduction

Recently the impact of plasma fluctuations in linear plasma machines on the sputtering process of exposed target material has been investigated by the use of synthetic turbulence to mimic the turbulent dynamics in a plasma beam [1]. This computationally efficient approach is based on the solution of Langevin equations describing plasma transport in a controlled fluctuating velocity field. The impact of the plasma fluctuations on the sputtering of particles from the target has been taken into account by a fluctuating sputter yield linearly related to the fluctuating flux of impinging ions. It is known that the complex structured plasma beam hitting the target material causes rich surface structures due to erosion processes. However, it is not clear to what extent the statistics of plasma beam changes the surface morphology compared to a homogeneous ion beam. In the present work the surface morphology is studied by the use of a Langevin equation of the Kuramoto-Sivashinsky type. In a first step the plasma fluctuations are put completely into the noise term of the Kuramoto-Sivashinsky-model.

Langevin Model for Plasma Turbulence

A fluid approach to describe the plasma transport has been employed in Ref. [1]. Electron density n_e and temperature T_e of the plasma containing singly charged ions end electrons evolve according to $\partial n_e/\partial t + V_\perp \cdot \nabla n_e = S_n - \nu_n n_e$ and $\partial T_e/\partial t + V_\perp \cdot \nabla T_e = S_T - \nu_T T_e$. Using the $E\times B$-velocity for the perpendicular velocity, i. e. $V_\perp = B \times \nabla\phi/B^2$ introduces a fluctuating piece due to fluctuating electric fields. For this purpose the electric potential ϕ is described by a 2D stochastic Langevin equation $\tau\,\partial\phi/\partial t = -\phi + \varepsilon\, Q(\zeta)$. The operator Q is a spatial filter on the Gaussian white noise ζ. The parameter ε is the amplitude of the noise and τ is the correlation time of the colored noise ϕ. The filter operator Q is assumed to be a functional of the perpendicular Laplacian $\nabla_\perp^2$=∇^2-$\nabla_\parallel^2$, where the $\parallel$ symbol denotes the direction along the magnetic field and perpendicular to the target surface. Similar to the method described in Ref. [2] the Fourier-decomposed filter is constructed by the choice of Fourier coefficients $Q_{m,n} = \exp\left[-\Lambda^2\left(m^2k_x^2 + n^2k_y^2\right)\right]$ with Λ representing the correlation length of the stochastic field ϕ. It is found that the Probability Density Function of the logarithmic electron density $\ln n_e$ in the passive scaler model system can be well described by a weighted sum of two Gaussians [1]. Consequently, the electron density n_e is distributed according to a double log-normal distribution.

Langevin Model for Ion Sputtering

In this work we study the interplay of the plasma beam and the surface morphology and aim to take into account details of the sputtering process. We focus on continuum models for the surface evolution during exposure to the plasma beam, namely variants of the noisy Kuramoto-Sivashinsky equation [3, 4, 5, 6, 7] which can be written as

$$\frac{\partial h}{\partial t} = v_0 - \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 - K \nabla^2 \nabla^2 h + \sigma \nabla^2 (\nabla h)^2 + \eta \tag{1}$$

where $\nu, K > 0$. The first term on the rhs is the constant erosion velocity v_0, the second term describes the relaxation of the interface due to surface tension ν. The third term is the generic non-linear term incorporating growth or erosion. The fourth term represents surface diffusion and the fifth term is an additional non-linear term which conserves the total mass at the surface. The last term on the rhs accounts for the statistics of the ion beam [7]. To derive such kind of model equation several ideas and physics models have been proposed in the literature. Here we mainly refer to the work of Muñoz-García et al. [3] and Lauritsen et al. [6]. The coefficients from Muñoz-García et al. are derived from analytical estimates and values from experiment for the linear phase and the stationary phase of nanopattern formation by ion-beam sputtering. The constant term v_0 and the noise η are neglected in these studies. In another study, Lauritsen et al. build a bridge to a microscopic model and derived the coefficients by analyzing a Master-Equation for particular surface processes. Their continuum model equation is also similar to Eq. 1 but with $\sigma = 0$. It is not completely clear how one can reconcile these two models using a different number of parameters and the question arises to what extent the ion beam noise η changes the evolution of morphology. In the model of Muñoz-García et al. the noise is not even present. It might be recommended to step back to a reasonable microscopic model as proposed in [6] or [8] to incorporate the plasma fluctuations in a straightforward way. In this work an ad hoc modification of the macroscopic model defined by Eq. 1 with $\sigma = 0$ is considered. We neglect the constant velocity v_0 and use the scaling $h \to \nu/\lambda\, h$, $x \to \sqrt{K/\nu}\, x$ and $t \to K/\nu^2\, t$ to find the basic model

$$\frac{\partial h}{\partial t} = -\nabla^2 h + \frac{1}{2} (\nabla h)^2 - \nabla^2 \nabla^2 h + \gamma \xi \quad , \quad \gamma^2 = \frac{5ab}{a_0} \frac{\lambda^2 K^2}{\nu^5} \tag{2}$$

where ξ is a correlated noise with log-normal distribution. The numerical sampling of ξ is done by computing $\exp(\zeta)$, where ζ is a correlated field computed according to the recipe described in Ref. [1] to obtain a field with mean value $\mu = 0$ and variance $\sigma^2 = 9/16$. Numbers for the parameters ν, K and λ might be chosen close to the values presented in Ref. [3] to receive an impression of typical dimensions: $\nu/\lambda = 1.70\,\text{nm}$, $\sqrt{K/\nu} = 3.88\,\text{nm}$ and $K/\nu^2 = 88.93\,\text{s}$. The additional parameters a, b and a_0 appearing in Eq. 2 for the noise amplitude γ have been introduced in [6] and are directly related to microscopic quantities. The parameter a denotes the lattice spacing in the target plane, b is the lattice spacing in normal direction and a_0 is a parameter describing the curvature dependence of surface erosion. The particular advantage of the re-scaled form of Eq. 2 is that only a single parameter is left, i. e. the noise amplitude γ.

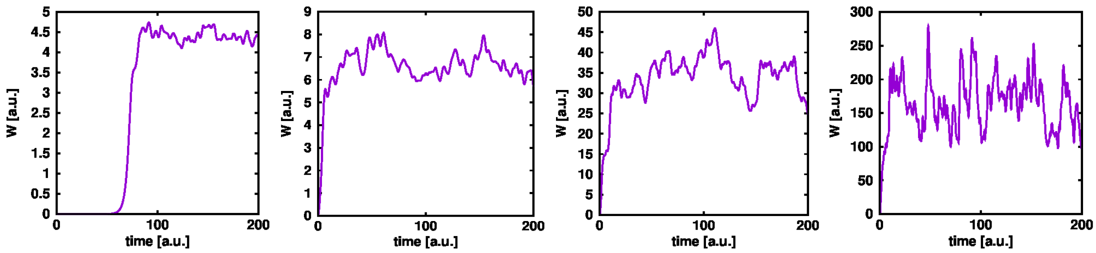

Figure 1: Time traces of the interface width W in units of $\sqrt{K/\nu}$ for the simulations with $\Lambda = \sqrt{K/\nu}$ and $\gamma = 0$, 1, 5 and 30 (from left to right). The time is given in units of K/ν^2.

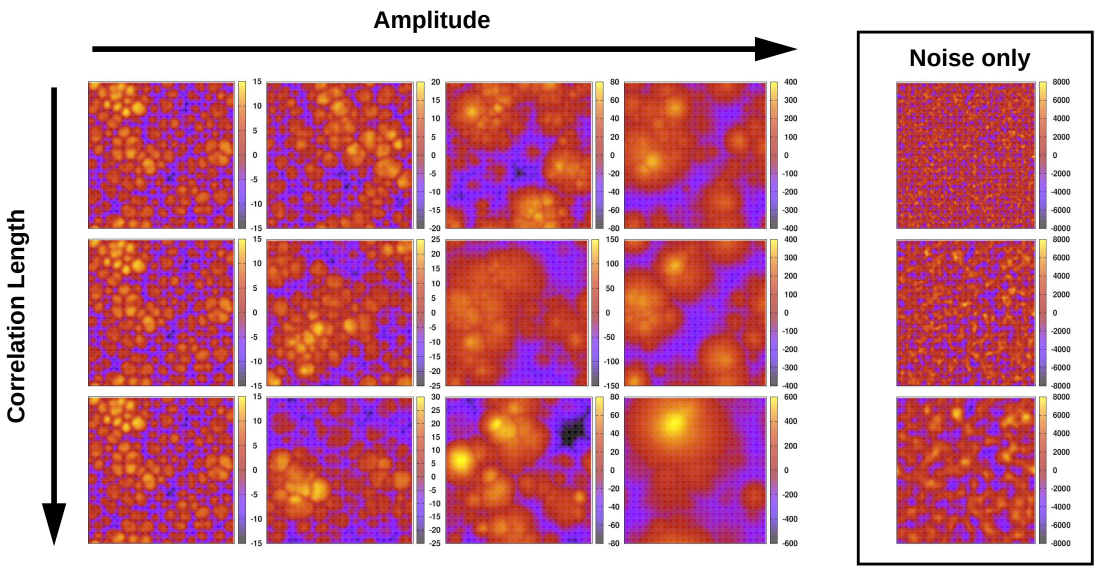

Figure 2: Patterns of height function h on a periodic $L \times L$ domain with side length $L = 100\sqrt{K/\nu}$ at time $t = 200\,K/\nu^2$. The twelve figures on the left show the patterns for correlation length Λ chosen as 1, 2 and 4 $\sqrt{K/\nu}$ (from top to bottom) and scaled noise amplitude $\gamma = 0$, 1, 5 and 30 (from left to right). The additional three figures on the right show the patterns for all terms switched off in the numerical simulation of Eq. 2 except the noise term.

Simulation Results

The numerical study consists of simulation runs for the system Eq. 2, where the noise amplitude γ is varied between 0 and 30 and for each value of γ the correlation length Λ is varied between 1 and 4 $\sqrt{K/\nu}$. An important parameter to study in the temporal evolution of the surface morphology is the interface width $W = \sqrt{\left\langle (h^2 - \langle h \rangle)^2 \right\rangle}$, where $\langle \cdots \rangle$ denotes the average over the two-dimensional computational domain. Each simulation run is tracked until the interface width W is statistically stationary. Examples of such time traces are shown in Fig. 1. For all combinations of parameters a statistically stationary state is obtained at time $t = 200\,K/\nu^2$. The resulting patterns of the height function h are shown in Fig. 2. The most obvious change in the surface structure is seen in for increasing noise amplitude. Whereas the correlation length of the noise does not really modify the structure for a given amplitude γ, the noise strength has a clear impact in coarsening the patterns. This result stems from all physics effects contained in Eq. 2 and not just from an increasing dominance of the noise. To demonstrate this, the right column in Fig. 2 shows the resulting patterns obtained by neglecting all other terms except the noise. There the resulting patterns do not show the pronounced coarsening obvious in the scan. The observed effect of the noise statistics is often not considered in detail and the most important step would be to sort out the effects of surface physics and plasma beam statistics in a rigorous mathematical model based on an appropriate microscopic stochastic description and a consistent derivation of macroscopic equations.

Acknowledgements

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