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Wavelet analysis of coarsening during unstable MBE growth

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Abstract

We present a wavelet analysis of coarsening of mounds during molecular beam epitaxy. The advantage in using wavelets over Fourier analysis is that one can track the coarsening process in both, location (direct space) and frequency (or scale) space at the same time. The wavelets concise scale decomposition allows the discrimination of the coarsening process, i.e. tracking coarsening at different scales.

Keywords: Wavelets; MBE growth; Coarsening; Continuum model

1. Introduction

Microelectronics technology has created an increasing interest in theoretical studies of molecular beam epitaxy (MBE) over the last few decades [1,2]. Many aspects of MBE growth were studied in a phenomenological framework. Phenomenological continuum models consider the surface of the growing film as a continuous variable of the position. Growth mechanisms, such as diffusion and desorption, can be introduced as functions of the surface height derivatives, provided that symmetry requirements are respected [3]. MBE growth can be summarized as follow: atoms are adsorbed on the film surface from the gas phase, where they undergo diffusion (which is thermally activated) or desorption back to the gas phase. The diffused adatoms will combine to other adatoms to form a dimmer, or will bind to steps of existing islands on the surface. A whole atomic layer is formed once all islands on the surface have coalesced. In an ideal situation, the growth proceeds in a layer-by-layer mode, resulting in atomically smooth surfaces. However, many experiments provide evidence that layer-by-layer growth mode do not occur in many practical situations [4,5]. The layer-by-layer mechanism may be suppressed by two other dominant effects: shot noise, or instabilities that arise from the so-called Ehrlich–Schwoebel (ES) effect [6,7]. Shot noise originates from different mechanisms such as deposition, diffusion or nucleation. The ES effect is due to the asymmetry in attachment–detachment kinetics across an atomic step, i.e. atoms have to overcome an energy barrier when descending a step. This favours an ascending atomic current, which is responsible for the instability of an initial flat surface against small perturbations. As a result, the amplitude of such perturbations will exponentially increase in time. This unphysical situation can be cured by introducing a stabilizing mechanism such as Mullins-like current arising from thermodynamic relaxation through surface diffusion [8] or from fluctuations in the nucleation process of new forming islands [9,10]. In a deterministic picture, one can neglect all noise sources; then growth can be treated considering only the ES destabilizing and Mullins stabilising currents. These two effects will induce the formation of a mound-like structure on the surface; the formed mounds will coarsen after an initial phase. So far, the analysis of the coarsening process has been performed globally, i.e. it describes the coarsening of mounds as a global process without taking into consideration how coarsening proceeds at different scales. The purpose of this paper is to make use of the wavelets formalism to analyse the coarsening process at different scales.

2. Basic equations

A phenomenological continuum model describing the surface growth incorporating this two conserving

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mechanisms can be formulated as

$$\frac{\partial h}{\partial t} = -\nabla \vec{j}_d - \nabla \vec{j}_s \quad (1)$$

where h is the surface height, ∇ is the gradient, j_d is the ES destabilizing current and j_s is the Mullins stabilizing current. A simple model for the currents j_d and j_s can be expressed as [11]

$$j_d = \nu m\left(1 - \frac{m}{m_0}\right), \quad j_s = K\nabla^2 m \quad (2)$$

where $m = \partial h/\partial x$ is the surface slope; ν and K are positive constants. The model for the destabilizing current j_d predicts the emergence of the so-called 'magic slope', i.e. the surface mounds approach a constant slope after a transient phase of steepening. Eq. (1) has been investigated by mapping it to the phase ordering problem [12] or by mapping it to a one-dimensional system of interacting kinks [13].

The scenario as predicted by Eq. (1) is the following: due to ES instability, the surface will evolve towards a mound like structure with a well defined period $L_c = \sqrt{2K/\nu}$. Later in time, the mounds will coarsen because of the non-linearity of the current j_d. The period of the mounds $L(t)$ will increase logarithmically. That is

$$L(t) = a \ln(t) + b \quad (3)$$

where a and b are constant coefficients. The surface slopes they will evolve towards the constant value $\pm m_0$.

3. Wavelet analysis

Wavelet analysis is the breaking up of a signal into shifted and scaled versions of the original (or mother) wavelet. That is

$$\psi_{s,x}(y) = \frac{1}{\sqrt{s}}\Psi\left(\frac{y-x}{s}\right) \quad (4)$$

where s ($s>0$) and x are the scale parameter and the dilatation parameter, respectively, y is the space variable, and Ψ is the mother wavelet. These basis functions vary in scale by slicing the data space using different scale sizes. The continuous wavelet transform (CWT) is defined as the sum over all of the surface profile multiplied by the shifted and scaled mother wavelet

$$W(s,x) = \int h(y)\psi_{s,x}(y)\mathrm{d}y \quad (5)$$

where $W(s,x)$ is the wavelet coefficient which is a function of the scale and the position. Then, CWT describes the surface profile in a given position x and a given scale s.

We start our analysis by discretizing Eq. (1) and solve it numerically in one dimensional space. Periodic boundary conditions are used (i.e. $h_1 = h_N$, where N is the system size). Then, the wavelet transform is performed using Eq. (5) at different times. In Fig. 1, we show a splitted surface profile generated from Eq. (1), and transformed using the transform (5), and the 'Mexican hat wavelet', for three different scales $s = 0.8$, 8 and 24 and for $t = 2$. Note that high oscillations correspond to small scales, while low ones correspond to large scales. Wavelets have the ability to split a surface profile up into components that are not pure sine waves, as opposed to Fourier transform. When summing all those components, one retrieves the exact profile.

Fig. 2 shows the evolution of the magnitude of the wavelet transform, for four different times: $t = 6$, 30, 40 and 70. At the early stage ($t = 6$), the wavelet power is concentrated within a band of scales, reminiscent of the instability leading to

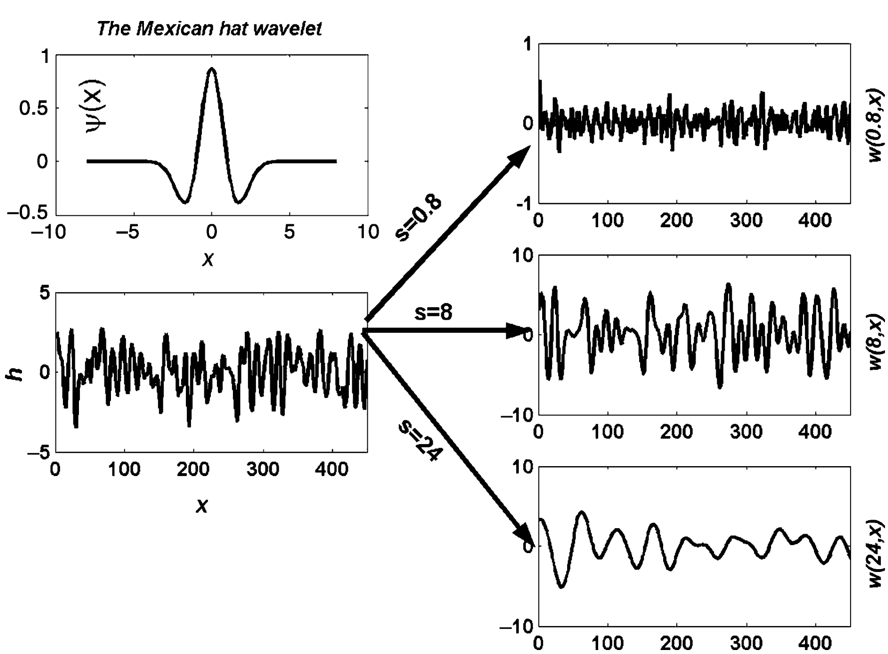

Fig. 1. The scale decomposition of the surface profile for $t = 2$ and for $s = 0.8$, 8 and 24. The 'Mexican hat' wavelet is used.

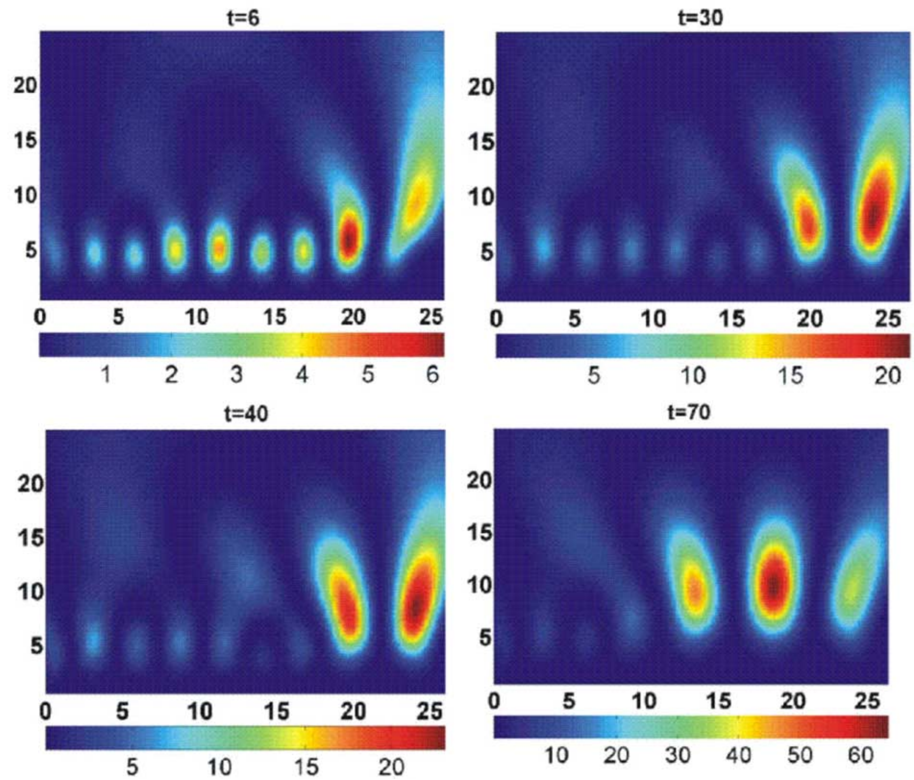

Fig. 2. The evolution of the magnitude of the wavelet transform of the surface profile, computed using Eq. (4), for $t=6$, 30, 40 and 70, showing the coarsening with increasing time.

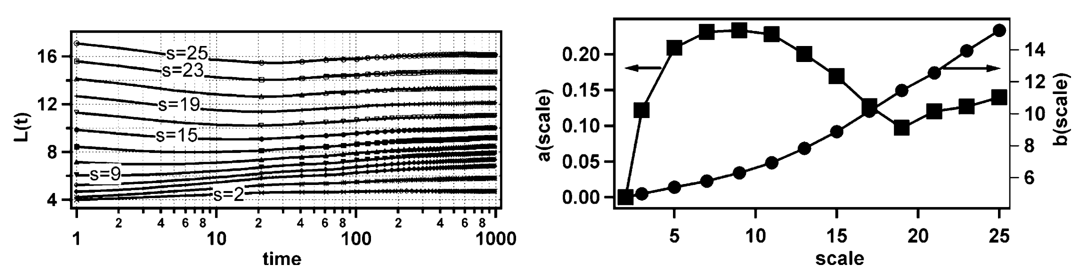

Fig. 3. Left: evolution of the surface feature size at different scales in log-linear plot, the integration parameters are $\nu=1$, $K=0.4$ and a system size of 1024 points. Right: the coefficients a(s) and b(s) for different scales

a dominate scale (or mound size $L=\sqrt{2K/\nu}$). Later in time, this band of scales shifts towards larger scales, an indication of coarsening.

In order to discriminate, the coarsening process, we compute the peak-to-peak distance $L_s(t)$ (the mound size), for each scale (or wavelet decomposition). The peak-to-peak distance is given by

$$L_s(t)=\frac{\int q|\tilde{W}(s,q)|^2\mathrm{d}q}{\int|\tilde{W}(s,q)|^2\mathrm{d}q} \tag{6}$$

where $|\tilde{W}(s,q)|^2$ is the Fourier power spectrum at a scale s and q is the wavenumber. Fig. 3 displays $L_s(t)$ for different scales. This figure shows three phases: the early stage with unstable growth phase, the transient phase and the coarsening phase. In the coarsening phase, the mound size varies logarithmically for all scales, i.e. $L_s(t)=a(s)\ln(t)+b(s)$. This means that the global logarithmic law (3) does not change with the scale. However, the coarsening speed a(s) is scale-dependent as shown in Fig. 3. The coarsening speed increases with the scale and reaches a maximum at $s\sim 8$, and decreases for large scales. In Fig. 3, the coefficient b(s) is also shown to increase with increasing scale. This is predictable since large scales correspond to large features.

4. Conclusion

In conclusion, an analysis of coarsening is performed using wavelets formalism. Wavelet formalism has an advantage over Fourier methods in a way that one can track the coarsening process in the location (direct space), and at different scales, simultaneously. We have shown that the global law of coarsening does not change with the scale, i.e. at all scales, the logarithmic law holds. Another important consequence of this analysis is that each scale coarsens with different speed. There exist a well defined scale where coarsening is the fastest.

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