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FORCED ANISOTROPIC MEAN CURVATURE FLOW OF GRAPHS IN RELATIVE GEOMETRY

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Abstract. The paper is concerned with the graph formulation of forced anisotropic mean curvature flow in the context of the heteroepitaxial growth of quantum dots. The problem is generalized by including anisotropy by means of Finsler metrics. A semi-discrete numerical scheme based on the method of lines is presented. Computational results with various anisotropy settings are shown and discussed.

Keywords: anisotropy; mean curvature flow; Finsler metric; fused deposition modeling; epitaxial growth

MSC 2010: 35K57, 35K65, 65N40, 53C80

1. Introduction

Heteroepitaxy is an important technology for today's electronic and photonic devices. Understanding the physics underlying epitaxial growth is crucial for the development of new and better devices. Here, we shall focus on the strain effect on the instability of island formation, known as the Asaro-Tiller-Grinfeld (ATG) instability [10]. The physical mechanism of this instability can be explained as follows. While a flat surface has the lowest surface free energy, a corrugated surface has lower elastic energy than the flat one. The elastic energy is lowered by elastic deformation so that the film breaks into isolated islands (called quantum dots). Therefore, the quantum dots are caused by the competition between surface and elastic energies. Elastic energy is reduced as the surface area increases. The surface morphology may also be affected by anisotropy in surface energy as it may reveal a faceted structure.

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We consider the evolution of a 2-dimensional surface $\Gamma(t)$ embedded in $\mathbb{R}^3$ representing the interface between the vapour and the thin film. Then, the equation of motion reads [9]

$$v_{\Gamma,\varphi} = D\Delta_s w, \tag{1.1}$$

$$w = \kappa_{\Gamma,\varphi} + \frac{1}{M}v + \Psi. \tag{1.2}$$

Here, $v_{\Gamma,\varphi}$ denotes the normal velocity, D a positive diffusion coefficient, Δ_s the Laplace-Beltrami operator, w the chemical potential, $\kappa_{\Gamma,\varphi}$ the anisotropic mean curvature, M a positive kinetic coefficient, and Ψ the elastic energy density.

Let us focus on the attachment-detachment dominated case. For $D \to \infty$, $M = 1$ the system (1.1)–(1.2) turns into the area preserving mean curvature flow [9]

$$v_{\Gamma,\varphi} = -\kappa_{\Gamma,\varphi} + f \text{ on } \Gamma(t), \tag{1.3}$$

where

$$f = \frac{\int_\Gamma \kappa_{\Gamma,\varphi}\,\mathrm{d}s}{\int_\Gamma \varphi^0(n_\Gamma)\,\mathrm{d}s} - \Psi + \frac{\int_\Gamma \kappa_{\Gamma,\varphi}\,\mathrm{d}s}{\int_\Gamma \varphi^0(n_\Gamma)\,\mathrm{d}s}, \quad \varphi^0 \text{ is a Finsler metric.} \tag{1.4}$$

The law (1.3) with $f = 0$ has been extensively studied. Deckelnick and Dziuk proved the convergence and gave the optimal error estimates using the finite element method for graph [3], [4] and parametric [5] case. Haußer and Voigt [6] presented a parametric finite element approximation for a regularized version. Pozzi studied the anisotropic mean curvature flow in higher codimension in [8].

In this paper, we study the graph formulation of the law (1.3). For this purpose, we assume that the interface is written as the graph of a scalar function p such that

$$\Gamma(t) = \{[x, y] \in \mathbb{R}^3;\ y = p(t, x),\ x \in \Omega \subset \mathbb{R}^2\}.$$

The main improvement of this work is the incorporation of the anisotropic mean curvature based on the Finsler geometry into the forced mean curvature flow (1.3). The numerical studies demonstrate the effect of the surface energy anisotropy on the self-assembled growth of quantum dots.

2. Anisotropy in relative geometry

In order to incorporate the anisotropy into the model we shall utilize the framework developed in [1] and used in e.g. [2], [7]. We say that a continuous function $\varphi\colon \mathbb{R}^3 \to \mathbb{R}_0^+$ is a Finsler metric if it satisfies the conditions

(1) $\varphi \in C^{3+\alpha}(\mathbb{R}^3 \setminus \{0\})$,
(2) φ^2 is strictly convex,
(3) $\varphi(t\eta) = |t|\varphi(\eta)$, $t \in \mathbb{R}$, $\eta \in \mathbb{R}^3$,
(4) $\lambda|\eta| \leqslant \varphi(\eta) \leqslant \Lambda|\eta|$, $\eta \in \mathbb{R}^3$, for two suitable positive constants $0 < \lambda \leqslant \Lambda < \infty$.

Associated with φ we define the unit ball (also called the Wulff shape)

$$B_\varphi = \{\eta \in \mathbb{R}^3;\ \varphi(\eta) \leqslant 1\}.$$

One can prove that the dual function $\varphi^0\colon \mathbb{R}^3 \to \mathbb{R}_0^+$, given by

$$\varphi^0(\eta^*) = \sup\{\eta^* \cdot \eta;\ \eta \in B_\varphi\},$$

is also a Finsler metric.

For simplicity we use η instead of η^*. Then the following relations hold:

$$\varphi^0_\eta(t\eta) = \frac{t}{|t|}\varphi^0_\eta(\eta),\ \ \varphi^0_{\eta\eta}(t\eta) = \frac{1}{|t|}\varphi^0_{\eta\eta}(\eta),\ \ t \in \mathbb{R} - \{0\},$$
$$\zeta \cdot \varphi^0(\eta)\varphi^0_{\eta\eta}(\eta)\zeta \geqslant \gamma_0|\zeta - \frac{\zeta\cdot\eta}{|\eta|^2}\eta|^2,\ \ \eta \neq 0,\ \zeta \in \mathbb{R}^n,\ \gamma_0 > 0,$$

where the index η means the derivative with respect to η.

We define the map $T^0\colon \mathbb{R}^3 \to \mathbb{R}^3$ as

$$T^0(\eta) = (\widetilde{T}^0(\eta), T^0_3(\eta)) = \varphi^0(\eta)\varphi^0_\eta(\eta) \quad \text{for } \eta \neq 0,$$
$$T^0(0) = 0.$$

Then, the φ-normal vector, φ-mean curvature, and φ-normal velocity of Γ are defined as

$$n_{\Gamma,\varphi} = \frac{T^0(\nabla p, -1)}{\varphi^0(\nabla p, -1)} = \varphi^0_\eta(\nabla p, -1), \tag{2.1}$$

$$\kappa_{\Gamma,\varphi} = \nabla \cdot n_{\Gamma,\varphi}, \tag{2.2}$$

$$v_{\Gamma,\varphi} = -\frac{\partial_t p}{\varphi^0(\nabla p, -1)}. \tag{2.3}$$

3. Equation of motion

By substituting the quantities (2.1)–(2.3) into Equation (1.3), we obtain the nonlinear parabolic partial differential equation

$$\partial_t p = \varphi^0(\nabla p, -1)\left(\nabla \cdot \frac{\widetilde{T}^0(\nabla p, -1)}{\varphi^0(\nabla p, -1)} - f\right) \text{ on } \Omega \times (0, T). \tag{3.1}$$

The initial and boundary conditions are given by

$$p|_{t=0} = p_0 \text{ on } \overline{\Omega}, \tag{3.2}$$

$$\frac{\partial p}{\partial n} = 0 \text{ on } \partial\Omega \times (0, T). \tag{3.3}$$

4. Numerical solution

For numerical solution, the method of lines is used. After approximating the spatial derivatives by finite differences we obtain the semi-discrete scheme

$$p_t^h = \varphi^0(\overline{\nabla}_h p^h, -1)\left(\nabla_h \cdot \frac{\widetilde{T}^0(\overline{\nabla}_h p^h, -1)}{\varphi^0(\overline{\nabla}_h p^h, -1)} - f\right), \tag{4.1}$$

where ∇_h, $\overline{\nabla}_h$ are, respectively, the forward and backward difference operators.

The initial condition is written as

$$p^h|_{t=0} = \mathcal{P}_h p_0.$$

The discretization of the Neumann boundary condition is defined as

$$\begin{aligned} p^h_{\bar{x}_1,1j} &= 0 \quad \text{for } j = 0, \ldots, N_2, \\ p^h_{\bar{x}_1,N_1 j} &= 0 \quad \text{for } j = 0, \ldots, N_2, \\ p^h_{\bar{x}_2,i1} &= 0 \quad \text{for } i = 0, \ldots, N_1, \\ p^h_{\bar{x}_2,iN_2} &= 0 \quad \text{for } i = 0, \ldots, N_1. \end{aligned}$$

The scheme can be rewritten in the general form

$$\frac{\mathrm{d}P^h}{\mathrm{d}t} = F(t, P^h).$$

Then, the Runge-Kutta-Merson method is used for solving this system of ODEs.

5. Numerical results

We use the scheme (4.1) to perform a range of computations for the following anisotropies with $n = \eta/|\eta|$:

▷ the 4-fold symmetry

$$\varphi^0(\eta) = (1 - 0.245(1 - (n_1^4 + n_2^4 + n_3^4)))|\eta|,$$

▷ the 6-fold anisotropy

$$\varphi^0(\eta) = \Big(1 - 0.037\Big(n_1^4 + n_2^4 + n_3^4 - \frac{3}{5}\Big) + 0.037\Big(3(n_1^4 + n_2^4 + n_3^4) + 66n_1^2n_2^2n_3^2 - \frac{17}{7}\Big)\Big)|\eta|,$$

▷ and the 8-fold symmetry

$$\varphi^0(\eta) = (1 + 0.0155(n_1^8 + n_2^8 + n_3^8 - 28(n_1^6n_2^2 + n_1^2n_2^6 + n_2^6n_3^2 + n_2^2n_3^6 + n_3^6n_1^2 + n_3^2n_1^6) + 70(n_1^4n_2^4 + n_2^4n_3^4 + n_3^4n_1^4)))|\eta|.$$

In all computations, the initial condition $p_0 = 1 + 0.01\cos(\pi x)\cos(\pi x)$ and the domain $\Omega = (0,2) \times (0,2)$ are used. The forcing term (1.4) is set with the prescribed elastic energy density $\Psi = 50/p$.

First, we show the quantitative solution analysis. We evaluate the experimental order of convergence (EOC) as

$$\mathrm{EOC} := \frac{\log(\mathrm{Error}_1/\mathrm{Error}_2)}{\log(h_1/h_2)},$$

where $\mathrm{Error_i} = \|p - p^{h_i}\|$, p is the numerical solution computed on the grid 800×800 substituting the analytical solution, p^{h_i} is the numerical solution computed on courser grid with mesh size h_i. The results are shown in Table 1.

N	h	Error L_∞	Eoc L_∞	Error L_2	Eoc L_2
50	1/25	0.02755	—	0.00642	—
100	1/50	0.01270	1.11722	0.00320	1.00252
150	1/75	0.00784	1.18235	0.00203	1.12392
200	1/100	0.00542	1.29443	0.00143	1.23257

Table 1. Experimental order of convergence of the scheme (4.1).

Figures 1–3 show the solutions at different times. Starting with almost flat interface we observe the surface instability which results in faceted quantum dots. The shape of quantum dots is determined by the corresponding anisotropy symmetry.

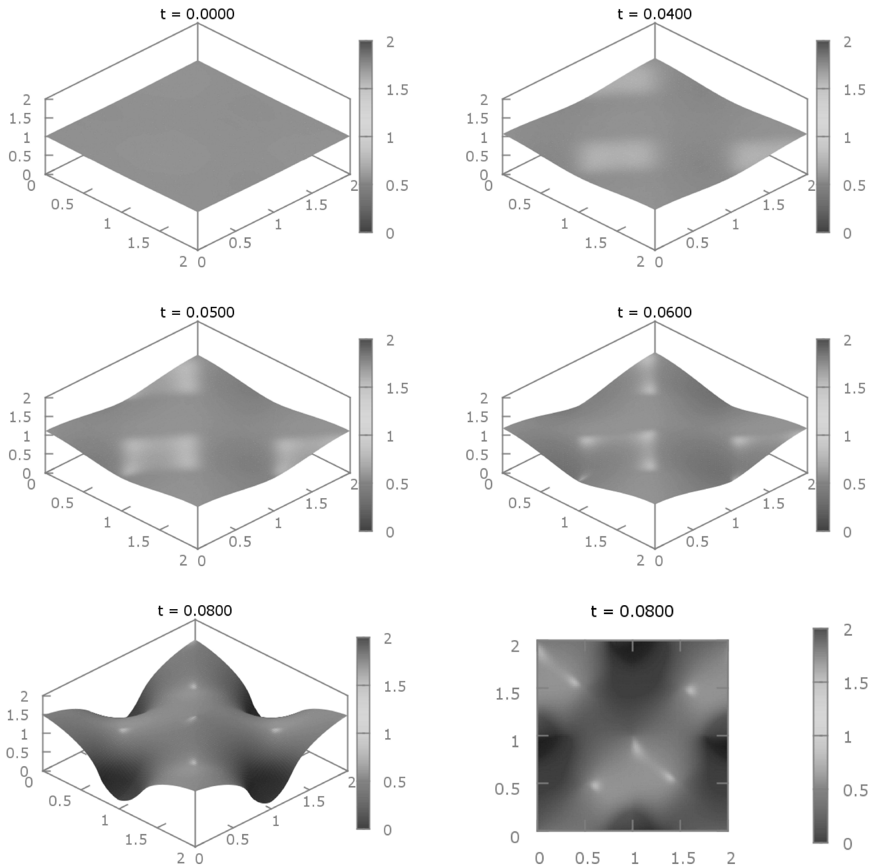

Figure 1. Surface evolution for the 4-fold symmetry anisotropy, space step $h = 0.01$.

6. Conclusion

In the paper, we have used the forced anisotropic mean curvature flow of graphs to model the ATG instability in the case where the attachment-detachment process is dominated. We have demonstrated numerical convergence of the numerical scheme based on the method of lines and presented numerical experiments showing the influence of various anisotropy symmetries on the surface evolution.

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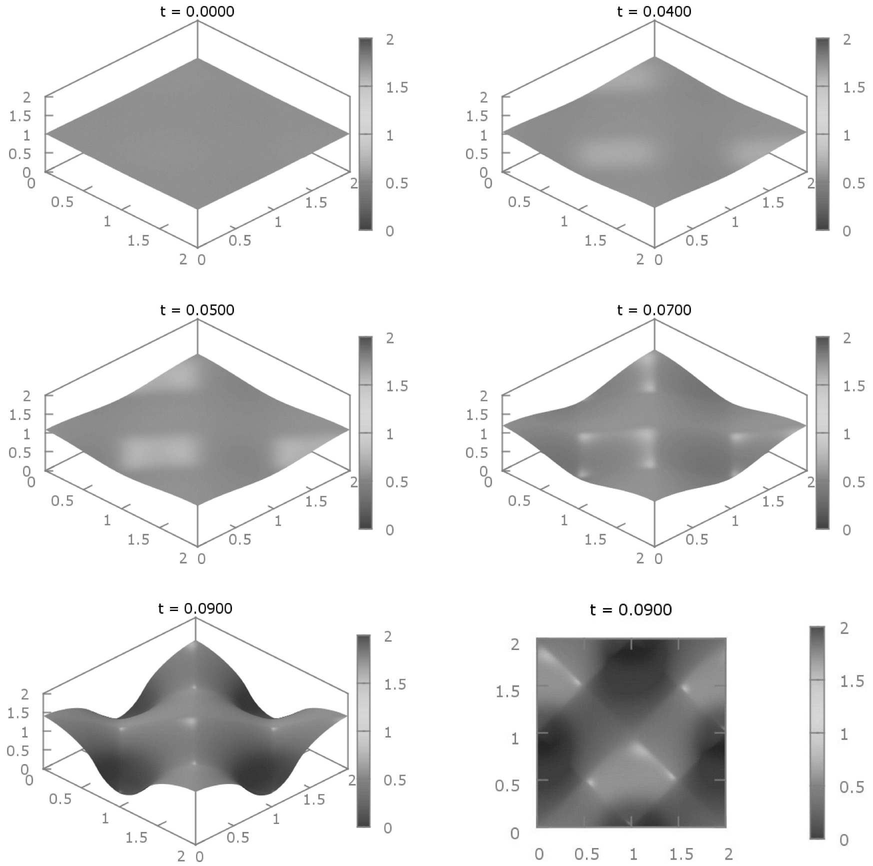

Figure 2. Surface evolution for the 6-fold symmetry anisotropy, space step $h = 0.01$.

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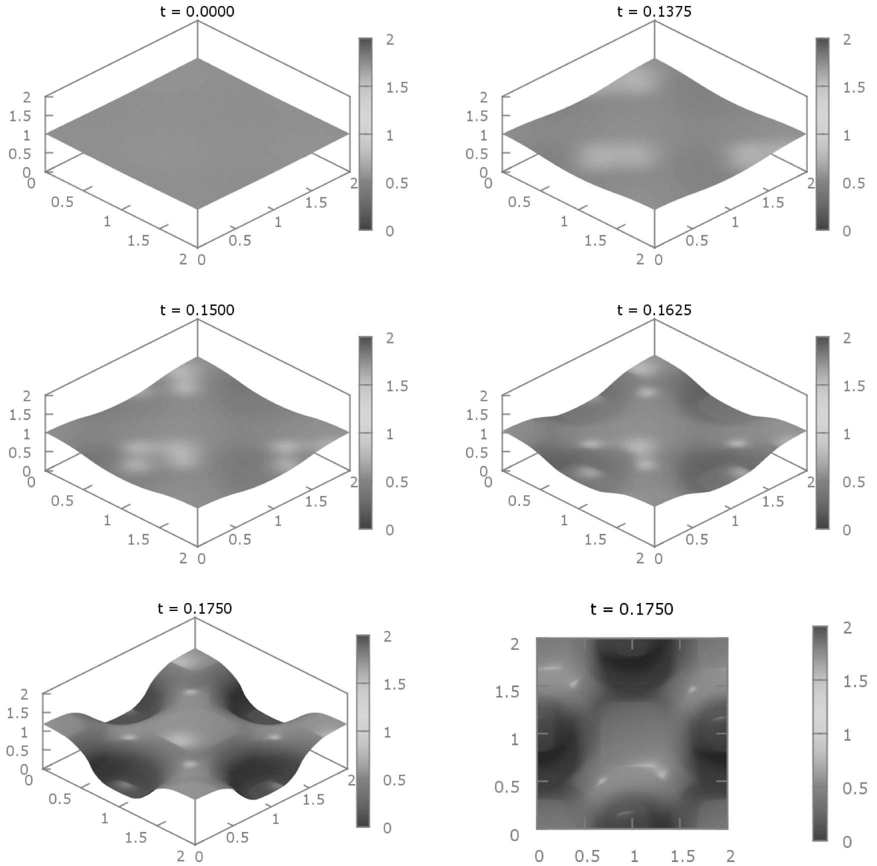

Figure 3. Surface evolution for the 8-fold symmetry anisotropy, space step $h = 0.01$.

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