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Existence, Uniqueness and Energy Scaling of (2+1)-Dimensional Continuum Model for Stepped Epitaxial Surfaces with Elastic Effects

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Abstract. We study the (2+1)-dimensional continuum model for the evolution of stepped epitaxial surface under long-range elastic interaction proposed by Xu and Xiang (SIAM J. Appl. Math. 69 (2009), 1393–1414). The long-range interaction term and the two length scales in this model makes PDE analysis challenging. Moreover, unlike in the (1+1)-dimensional case, there is a nonconvexity contribution in the total energy in the (2+1)-dimensional case, and it is not easy to prove that the solution is always in the well-posed regime during the evolution. In this paper, we propose a modified (2+1)-dimensional continuum model based on the underlying physics. This modification fixes the problem of possible illposedness due to the nonconvexity of the energy functional. We prove the existence and uniqueness of both the static and dynamic solutions and derive a minimum energy scaling law for them. We show that the minimum energy surface profile is mainly attained by surfaces with step meandering instability. This is essentially different from the energy scaling law for the (1+1)-dimensional epitaxial surfaces under elastic effects attained by step bunching surface profiles. We also discuss the transition from the step bunching instability to the step meandering instability in (2+1)-dimensions.

AMS subject classifications: 70G75, 70K42, 70K50

Key words: Epitaxial growth, elastic effect, energy scaling law, step bunching instability, step meandering instability.

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1 Introduction

In epitaxial film growth, elasticity-driven surface morphology instabilities have been widely employed to generate self-assembled nanostructures on the film surfaces, which exhibit interesting electronic and optical properties and have various applications in semiconductor industry [26, 28]. In heterogeneous epitaxial film, the film has a different lattice constant than that of the substrate, and the misfit strain causes step bunching and step meandering instabilities on such a surface. It is important to understand these instability phenomena due to elastic effects for the design and fabrication of advanced materials based on the self-assembly techniques.

In practice, most semiconductor devices are fabricated on vicinal surfaces when the temperature for epitaxial growth is below the roughening transition. In this case, these surfaces consist of a succession of terraces and atomic height steps. Traditional continuum models [2, 14, 31] that treated the surface as a continuum cannot be applied directly. Tersoff *et al.* [34] proposed a discrete model that describes the dynamics of each step. In their model, the elastic interactions between steps include the force dipole caused by the steps and the force monopole caused by misfit stress. The force dipole stabilizes a uniform step train while the force monopole destabilizes it, leading to the step bunching instability. Duport *et al.* [4] also proposed a discrete model to account for these effects. Besides the dipole and monopole interactions, their model includes the elastic interactions between the adatoms and steps as well as the Schweobel barrier. In (2+1)-dimensions, the elastic effects also lead to step meandering instability that competes with the bunching instability for straight steps, and these instabilities and their competitions have been examined by Tersoff and Pehlke [33], Houchmandzadeh and Misbah [15], and Leonard and Tersoff [19] using discrete models.

Xiang [35] derived a (1+1)-dimensional continuum model for the stepped surfaces with elastic effects by taking the continuum limit from the discrete models [4, 34]. Instability analysis and numerical simulations based on this continuum model performed by Xiang and E [36] showed that this continuum model is able to correctly describe the step bunching instabilities compared with the results of discrete models and experimental observations. Xu and Xiang [37], Zhu *et al.* [38] further developed a (2+1)-dimensional continuum model for the stepped surfaces with elastic effects, which is able to account for both the step bunching and step meandering instabilities as well as their competition. Kukta and Bhattacharya [18] proposed a three-dimensional model for step flow mediated crystal growth under stress and terrace diffusion. There are also continuum models for the surfaces in homoepitaxy, which contain only the force dipole elastic effect, e.g., [16, 20, 25, 29].

Luo *et al.* [22] analyzed the step bunching phenomenon in epitaxial growth with elasticity based on the Tersoff's discrete model [34]. In this work, a minimum energy scaling law for straight steps was derived and the one bunch structure was identified. They further extended the analyses to one-dimensional discrete system with general Lennard-Jones type potential [23] as well as one-dimensional continuum model with gen-