Modeling of Anisotropic Surface Energies for Quantum Dot Formation and Morphological Evolution

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Abstract:

Quantum dots are nanoscale structures that can be formed during heteroepitaxy of a thin film onto a substrate. These dots form as a result of the lattice misfit (the difference between the lattice parameters of the film and the substrate materials), which results in strain. Quantum dots exhibit distinctive properties, such as electrical properties, which have proven useful in recent advances in nanotechnology, resulting for example in quantum dot lasers, and could enable further advancements in electronics and computing. The purpose of this project is to build a mathematical framework for describing the anisotropic surface energies to be implemented in the simulations of growth of quantum dots and other relevant materials.

In the first part of the project, the commercial program, Mathematica®, was used to find mathematical descriptions of anisotropic surface energies with various symmetries that are expected from the underlying crystallographic structure of materials. Two-dimensional descriptions of the surface energies were created first, which were then extended to three-dimensional descriptions. After the mathematical formulas of the descriptions were obtained, the equilibrium shapes, or Wulff shapes, associated with these surface energies were calculated and visualized, again using Mathematica®.

Introduction:

Quantum dots can be formed through a variety of different processes. This project focused on modeling the energy anisotropy for the quantum dots formed through a process known as heteroepitaxy, a process in which a thin film of one material, such as germanium, is deposited on a substrate of another material, such as silicon. There is a lattice misfit between the film and the substrate due to the difference in the lattice parameters of the two materials, which results in strain. The formation of quantum dots is the result of the system attempting to minimize the total energy—the interfacial energy and the strain energy.

Surface energy anisotropy contributes to the manner in which quantum dots self-assemble. It has been found that the kind of surface energy anisotropy that the system has, greatly influences the way that quantum dots grow and configure themselves [1].

Information obtained in experiments can be used to model the interfacial energy anisotropy for actual crystal systems. For example, for a metal alloy AlSn, Napolitano and Liu grew crystals experimentally, then measured the equilibrium shapes for the liquid droplets entrained in the crystalline phase [2]. Given these equilibrium shapes, they extracted the interfacial free energy anisotropy as a mathematical function and parameters to fit the experimental result. The equilibrium shapes of crystals grown in semiconductor systems can also be measured and used to model the surface energy anisotropy using similar means.

Methods:

Mathematical models of various anisotropic surface energies were first obtained. Two-dimensional descriptions of surface energies as functions of the direction of the surface normal were created to have various symmetries. These two-dimensional surface energy descriptions were expressed in polar coordinates and plotted using Mathematica®. Then, trigonometric identities and other mathematical methods were used to extend these two-dimensional descriptions into equivalent three-dimensional descriptions (as functions of three normal components) to model the anisotropic surface energies of three-dimensional crystals. The surface energies with various degrees of anisotropy were visualized by writing the normal components in spherical coordinates and plotting them using Mathematica®.

These three-dimensional surface energy descriptions can then provide the corresponding equilibrium shapes of the crystals using a process called Wulff construction. Geometrical, Wulff construction involves drawing a plane perpendicular to each normal unit vector on the energy graph; the inner envelope formed by these planes is the equilibrium shape. We instead used the plot $\xi = \gamma n + \gamma_\theta \theta + \gamma_\varphi \phi$ [3] to visualize the equilibrium shapes in spherical coordinates.

Results:

Using Mathematica® for plotting, equilibrium shapes were modeled with different degrees of anisotropy for energies with four-fold, eight-fold, and twelve-fold symmetries in the three principle planes. Results are shown in Figures 1-4. "Ears" and "flaps" are present on equilibrium shapes associated with high degrees of anisotropy. These ears and flaps are also called missing angles. These equilibrium shapes approach shapes such as an octahedral in the case of four-fold symmetry; the equilibrium shapes of actual systems will not display these missing angles seen in the ears and flaps. Nonetheless, it is still important to examine such models because these anisotropic interfacial energies with missing angles model the facets of crystals.

Conclusion:

In this project, a mathematical framework was developed for modeling the anisotropic surface energies with various symmetries expected in the structures of various material systems. Two-dimensional energy descriptions were obtained, which were then extended to three-dimensional models. The equilibrium shapes associated with these three-dimensional surface energy models were obtained for different degrees of anisotropy. The descriptions obtained in this project will be used in simulations of the growth and the morphological evolution of quantum dots and their arrangements during heteroepitaxy.

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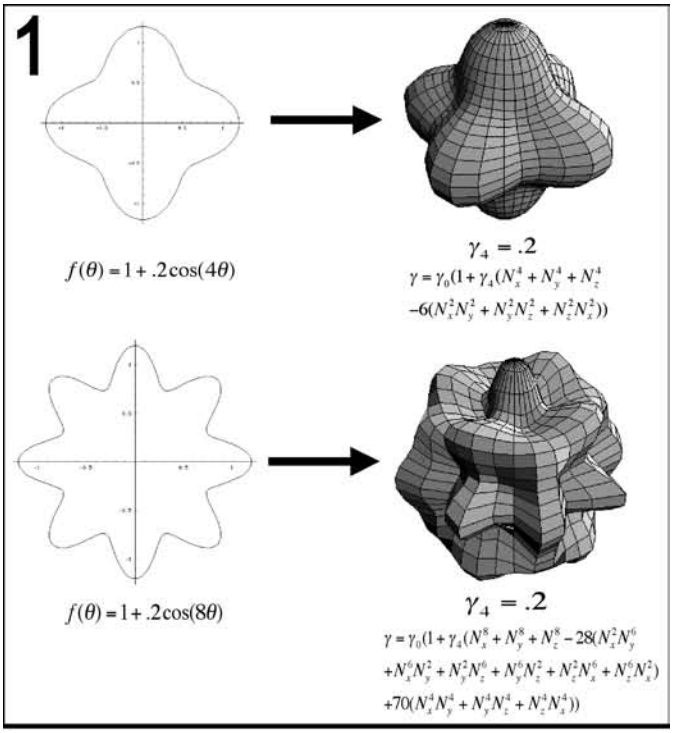

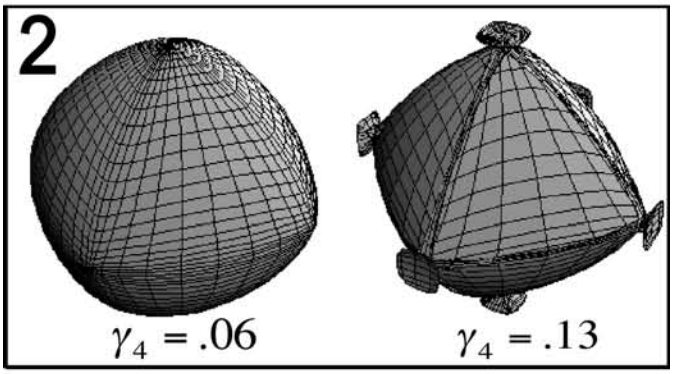

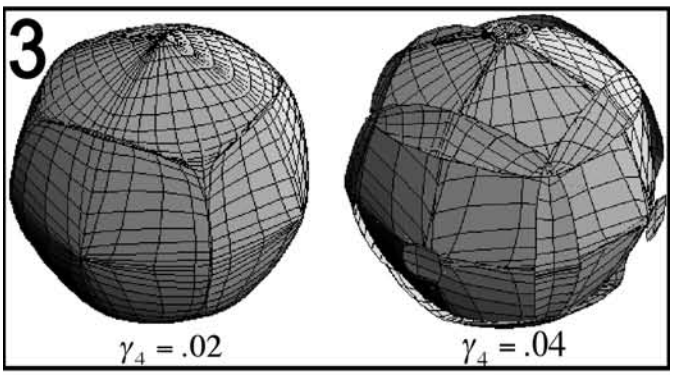

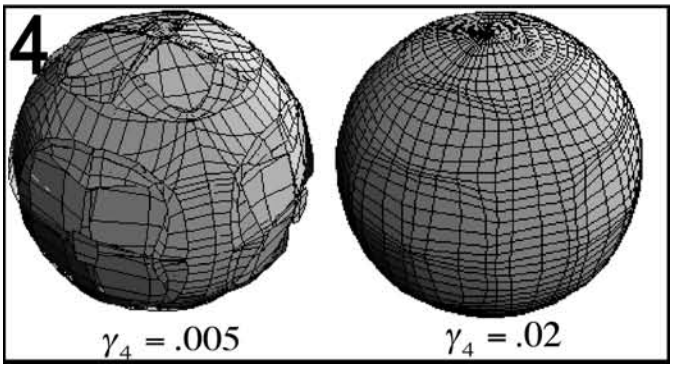

Figure 1: Anisotropic surface energy models in 2D and 3D with four-fold and eight-fold symmetry.

Figure 2: Equilibrium shapes for four-fold symmetry.

Figure 3: Equilibrium shapes for eight-fold symmetry.

Figure 4: Equilibrium shapes for 12-fold symmetry.