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RESEARCH STATEMENT

I am interested in numerical mathematics and probability. My research has been in the area of numerical math. I did a master's project involving phase fields, and my doctoral research involved the more detailed phase field crystal (PFC) model.

Doctoral Research

For my doctoral work, I applied the multimode PFC model with a vapor phase field to simulate the growth and layering of graphene (honeycomb geometry). In particular, I focused on the growth of graphene on a copper substrate, along with two-layer graphene development. My second major focus was the investigation of the surface energy generated by the solid-vapor phase interface. I examined four different facets, including armchair and zigzag (one- and two-bond stages).

The simulations employ the pseudo-spectral method in two-dimensional space, using a first order implicit and explicit (IMEX) time stepping scheme. The computational box is rectangular in R^2, which forms a periodic tiling of therein. I developed and ran the simulations in the MATLAB programming environment.

The PFC model operates on a diffusive time scale (freezing or melting) and an atomic length scale (crystal structures). Rather than discrete atomic positions, the model yields atomic probability densities. The density field is continuous, and areas of greater density indicate the most likely positions for atoms. By design, free energy decreases toward equilibrium over time. For most simulations, density (mass) is conserved.

The model revolves around a free energy integral. The integrand, or free energy density, includes polynomial terms that establish mass diffusion and a gradient term that generates crystal geometry. The gradient term employs a linear differential operator made up of Laplace transforms of various degrees.

By manipulating the gradient term, various crystal structures, such as triangular, honeycomb (graphene), and square geometry are possible. Because I employed the pseudo-spectral method for the discretization of the time derivatives, I studied the effects of the linear operator in Fourier space. In Fourier space, the linear operator becomes a polynomial multiplier. For honeycomb geometry, the polynomial has local minima at angular frequencies 1, sqrt(3), and 2. I learned to manipulate the polynomial to control crystal geometry and improve its stability.

As an alternative to a differential operator, I developed a system using a two-point correlation function to establish crystal geometry. In Fourier space, for honeycomb geometry, this correlation function becomes the sum of three Gaussian curves. As with the gradient approach, the locations and depths of the local minima determine the geometry.

I also studied the binary PFC model. This model incorporates two triangular PFC density fields, which, when superimposed, form honeycomb geometry.

Future Work

In the future, I hope to add a height function to the graphene model to simulate substrate delamination, and I wish to adapt the model to include a temperature field. In the combined fields of numerical math and probability, I aspire to study the modeling of Brownian motion.