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Simulation of Chemical Vapor Deposition for Graphene using Phase Field Crystal Models

The unique physical properties of graphene have been causing huge interest from both the fundamental scientific and application-oriented point of view. However, the potential of graphene remains hidden for future application unless a synthesis strategy has been established yielding large-area graphene films of sufficient purity. In this context, chemical vapor deposition (CVD) has been shown to be a promising bottom-up method in terms of scalability and reliability [1].
CVD-synthesis of graphene has already been successfully demonstrated, although there is still need for improvement regarding better quality. Since graphene films produced through CVD exhibit a polycrystalline structure, a lot of experimental effort have been made to control, for instance the domain size, the number of layers, the grain boundary density, and defects [2].
We are looking on challenges of CVD process for graphene production from a theoretical point of view. Here we present the phase field method as a powerful tool to simulate the time-resolved graphene growth on large scales, and thus to mathematically model the CVD process with the aim to find optimal process parameters. The idea of the phase field method is related to classical density functional theory in which the considered system is mapped by a continuously varying density field. The time evolution of the corresponding density is given by the variation of a free energy functional with respect to that density.
To model the CVD growth of graphene on metallic substrates, we construct an appropriate energy functional within three steps: (i) we apply the phase-field-crystal (PFC) model [3] which leads to an equilibrium density with a periodic honey-comb lattice (ii) we simulate the coexistence between a solid and gas phase using the vapor-PFC model [4] and (iii) we consider the substrate through an external pinning-potential [5].
First applications of our PFC-model are shown for the formation of grain boundaries of two graphene layers growing towards one another at different tilt angles, and the epitaxial growth of a graphene flake on a crystalline surface of different orientations which shows similar growth shapes compared to CVD experiments.

References

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Figures

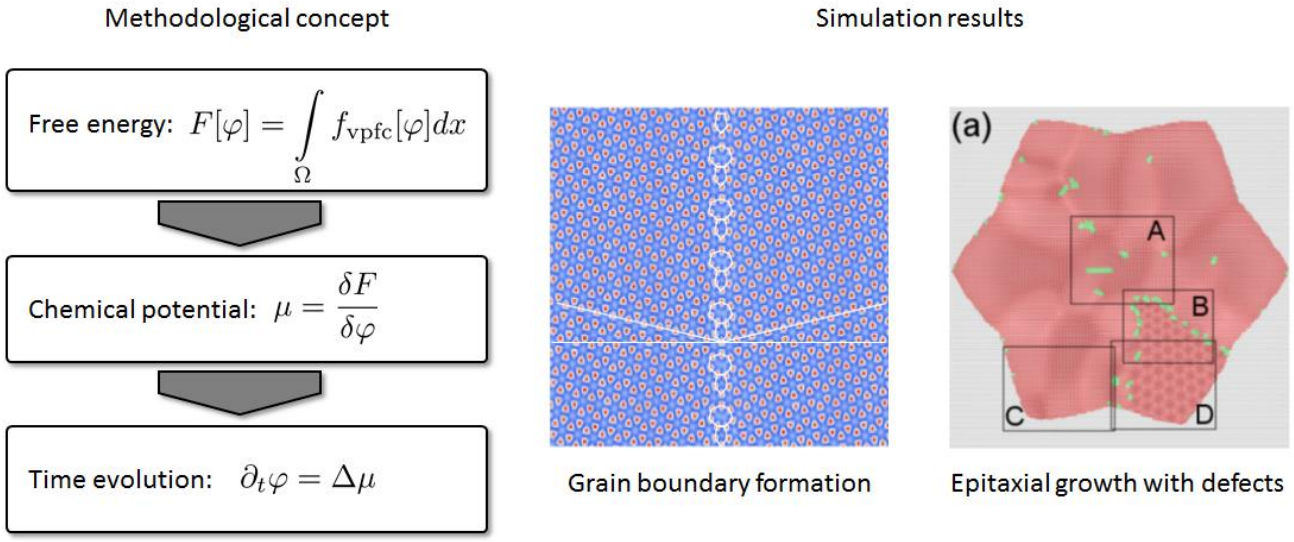

Figure 1: Left: Methodological concept of the phase field simulation. Right: Grain boundary formation exhibiting 5-7-ring defects and large-scale epitaxial graphene growth, both simulated by using the phase field method.