Grain boundary formation in two-dimensional materials

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The design of two-dimensional materials with controlled physical properties requires a precise control of their defects. For epitaxially grown two-dimensional materials such as graphene, the most important defects are grain boundaries, which control basic physical properties like electrical or thermal conductivities [1,2]. However, while many studies have allowed one to identify the mechanisms by which two-dimensional domains (or flakes) are nucleated, and grow, the formation of grain boundaries due to the collision of the edges of two growing flakes is still poorly understood.

In this study, we report on the modeling of the formation of grain boundaries in two-dimensional materials based on a combination of Kinetic Monte Carlo (on lattice) and analytical models (based on a Langevin model). Our models include energetic properties, such as interactions between the two edges [3] and edge line-tension, and kinetics of elementary mass transport processes, such as diffusion and attachment-detachment of growth units at the edges.

We find that the roughness of the grain boundaries emerging for the collision of the two edges during the growth process exhibits a non-trivial behavior, which combines equilibrium and non-equilibrium statistical fluctuations and morphological instabilities. We have obtained a global diagram of different regimes as a function of relevant physical parameters such as the growth rate, or kinetics of attachment at the edges. For example, in some conditions, the grain boundary roughness can be smaller for larger growth rates. Our study lays a theoretical framework to rationalize the control of grain boundary roughness in expitaxially grown two-dimensional materials.

References

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Figures

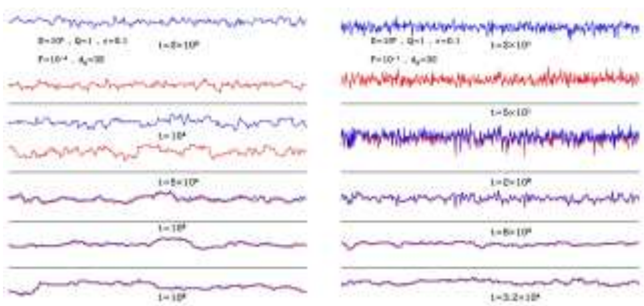

Figure 1: Simulations of the collision of 2 interfaces growing at low speed (left) and fast speed (right)