Dislocations in 2D: blessing or curse?

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Abstract

Dislocations in 2D systems were first observed several decades ago in the famous bubble raft experiment [1]. Currently, 2D materials like graphene, h-BN, and transition metal dichalcogenides offer a rich variety of problems for theory, with some key potential applications. Indeed dislocations are always present in materials and are usually undesirable because they can alter the electronic properties of the target material. A classical way to approach dislocations in 3D heterostructures is found in semiconductor science, where the presence of misfit dislocations can be avoided using the critical thickness framework introduce by Matthews and Blakeslee [2]. Here we recast this classic framework to consider interface misfit dislocation formation in 2D in-plane heterostructures [3]. We consider graphene-h-BN interfaces with various dislocation core reconstructions. This makes it possible to reveal a design space where defect-free heterostructures can be grown (see figure below). In other cases, dislocations might also be desirable, as they are building blocks for strengthening of materials through pile-ups that form grain boundaries. We will use the related framework of recrystallization to propose a way to tailor the properties of graphene. Here, using a modified hot-filament-assisted Chemical Vapor Deposition setup, which does not require any control of crystal nucleation and orientation. We propose an original growth mechanism [4] that includes a stage of structural evolution from nanocrystalline to microcrystalline graphene film opening a new route to control the electrical properties of large-scale uniform graphene film.

References

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Figures