2DHetero: hBN/Graphene 2D Heterostructures: from scalable growth to integration

Main area: Synthesis and characterization of layered materials beyond graphene
Keywords: hBN, MBE, CVD, growth mechanisms, theoretical simulations
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Abstract

Graphene is a 2D material, famous for its exceptional electronic properties. However, to exploit these properties in real devices, the electronic coupling with the substrate and with any surrounding material must be strongly reduced. Hexagonal boron nitride (hBN), another 2D material, is very promising for this purpose. It could be used both to insulate graphene from the substrate and as a gate dielectric material. Although devices obtained by mechanical exfoliation and transfer did confirm the strong potentialities of graphene/hBN heterostructures, a scalable and reliable growth technique remains to be demonstrated: the development of new approaches to the fabrication of 2D heterostructures is of high importance. By combining the know-how and resources of the project partners, the aim of the proposed study is to explore and develop various ways to fabricate graphene/hBN heterostructures on substrates compatible with Si microelectronics. Towards these goals, graphene/hBN heterostructures will be grown by two major methods: molecular beam epitaxy and chemical vapor deposition. The process may be improved by specific nucleation-enhanced lateral patterning to be developed in the course of the project. Advanced microscopy and spectroscopy techniques will be applied to provide information on the morphological, crystallographic, chemical and electrical properties of the films. Atomistic calculations by ab initio density functional theory complemented with large scale kinetic Monte Carlo simulations will be conducted to understand the growth mechanisms and optimal process conditions.

Moreover, while keeping in mind the ultimate goal that goes beyond this project, i.e., the growth of such heterostructures for device applications, the studies will result in the disclosure of the nucleation and growth mechanisms specific to hBN on graphene and to graphene on hBN. Such mechanisms should be generalized to generic Van der Waals (VdW) systems, to which both hBN and graphene belong. This will be made possible by performing the experiments on VdW substrates obtained in various ways and thus containing various types of nucleation centers, and by in-depth examination of typical samples by advanced imaging techniques augmented by theoretical calculations to elucidate the details of the chemical reactions involved and to simulate the growth. To understand the mechanisms is not only of fundamental scientific interest, but it is as well important for further development of graphene/hBN and similar systems. The experiments will be carried out on CMOS compatible materials, making this study unique, as its results might directly pave the way to the further graphene/hBN integration and device prototyping within the mainstream Si technologies.

Consortium

Mindaugas Lukosius – IHP GmbH – Leibniz Institut für innovative Mikroelektronik –Germany – Funded by: DFG
Jean-Francois Colomer – University of Namur – Belgique – Funded by: F.R.S.-FNRS
Dominique Vignaud – IEMN Institute of Electronics, Microelectronics and Nanotechnology – France – Funded by: ANR