Charge Transport in Polycrystalline Graphene-based Materials

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Graphene has attracted significant interest both for exploring fundamental science and for a wide range of technological applications. Chemical vapor deposition (CVD) is currently the only working approach to grow graphene at wafer scale, which is required for many industrial applications (flexible and transparent electrodes, RF devices, Hall sensors, photonics and optoelectronics, medical devices, nano-oscillators, etc.). Unfortunately, CVD graphene is intrinsically polycrystalline, with pristine graphene grains stitched together by disordered grain boundaries, which can be either a blessing or a curse. On the one hand, grain boundaries are expected to degrade the electrical and mechanical properties of polycrystalline graphene, rendering the material undesirable for many applications.

In this talk, I will describe fundamental properties of charge transport in disordered graphene and hybrids (chemically reduced, polycrystalline graphene, chemically functionalized, mixture of graphene and hBN, etc) of interest for currently explored and envisioned applications. The crucial contribution of high performance multiscale simulation will be shown, demonstrating high level of predictive capability for very large system sizes (with up to 1 billion atoms), reaching the experimental and technology scales, and therefore providing unique enabling tools for predicting or understanding complex phenomena occurring in two-dimensional membranes [1].

One will focus on the quantitative analysis on the transport properties of structural imperfections produced during the wafer-scale production of graphene, or the mechanical/chemical exfoliation and chemical transfer to versatile substrates, followed by the device fabrication. Fundamental properties of charge mobilities in polycrystalline graphene will be presented accounting the variability in average grain sizes and chemical reactivity of grain boundaries as observed in real samples grown by CVD will be presented [2,3,4], together with their relevance for device optimization and diversification of applied functionalities such as (bio)-chemical sensing.

The impact of grain boundaries (GBs) in the quantum Hall regime will be also addressed, with evidences for anomalous dissipation conveyed by the network of GBs, which provide pathways for electrons to circumvent field-induced localization [4,5].

The results presented here suggest interesting directions for utilizing grain boundaries to design sensors for detecting gases and molecules under different environmental conditions. As revealed by joint numerical and experimental measurements, the transport properties of grain boundaries can be strongly altered with chemical modifications of the grain boundaries. Together with highly conductive graphene, electrobiochemical sensing devices with high sensitivity and selectivity could be designed. Membrane science is another open research area. Although the ideal hexagonal graphene lattice impedes the diffusion of gases, defect sites such as heptagons, octagons, vacancies, and divacancies allow selective diffusion of limited gases and molecules, as mentioned above. This provides new opportunities to explore ultrathin membrane performance via the controlled engineering of grain boundaries and point defects.

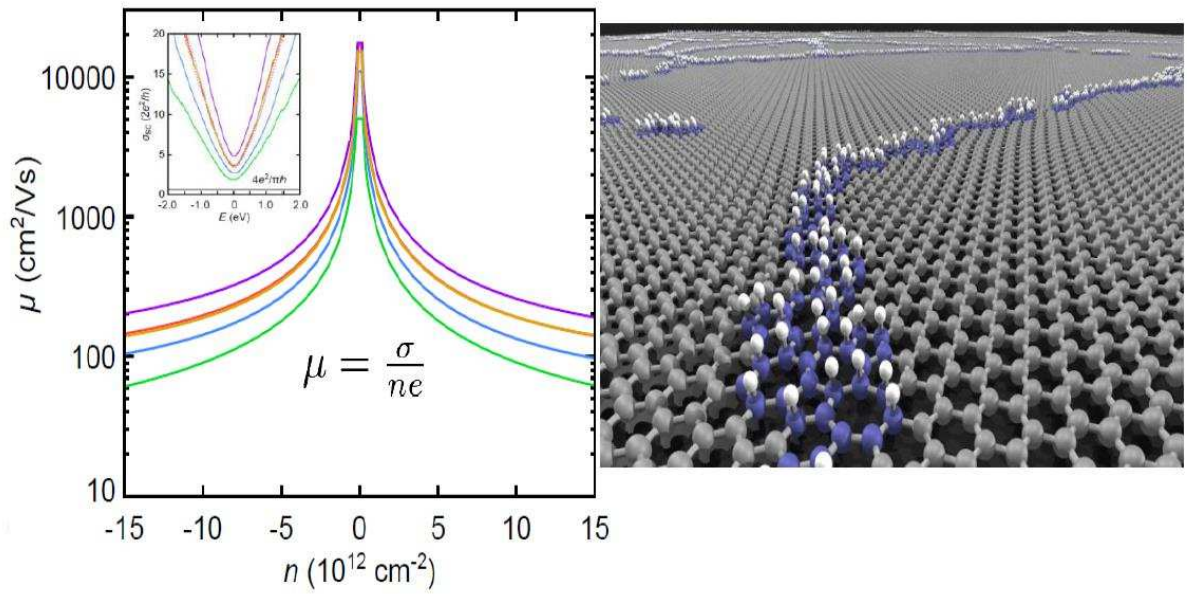

Figure 1: Left. Simulated charge mobility versus charge density in polycrystalline graphene models. Right: Ball-and-stick model of a polycrystalline graphene sample with grain boundaries chemically functionalized by hydrogen atoms.

References

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