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Atomic scale dynamics and modifications of stacked heteronanostructures under extreme conditions

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Abstract:

Since the discovery of atomically thin graphene, low-dimensional materials are making rapid progress for their use in future technology due to their exceptional intrinsic properties. Atomically thin nature of materials allows us to extrinsically introduce atomic scale modifications, hence manipulate the properties for particular application. The external manipulation processes are also important for optimizing the materials sustainability in device operations. There is a broad range of methods to externally modify materials, for example, the application of electric field, high temperatures, gaseous and liquid environment, electron and particle irradiation etc. The high-end electron microscopes with ˚A-level resolution and customized with tools made it possible to study the atomic structure of materials and test them under various environments which provide insights into structural dynamics and transformation of materials.

This thesis presents the structural modifications in 1D (carbon nanotubes), 2D (graphene, MoS_2) and their stacked systems under external stimuli such as electric biasing, plasma and highly charged ion irradiation by employing scanning transmission electron microscopy (STEM). In this thesis, I modified the target materials using various methods and performed *in situ* and *ex situ* experiments for observing the structural dynamics and evolution. Firstly, we used Ar plasma irradiation method to substitute heteroatoms (Si) in both graphene and SWCNTs lattices. The results reveal that the Si atoms are found in 3-fold and 4-fold configurations in SWCNTs. Secondly, we studied the effect of highly charged ions on graphene-MoS2heterostructrues. The results show that irradiation leads to the creation of nanosize pores in MoS2, while graphene lattice remains intact. In an experiment, when sample is irradiated on graphene side, both lattices remain unaffected. Finally, we performed *in situ* Joule-heating experiments on graphene and graphene-MoS_2 heterostructrues. The results exhibits dynamics, transformation and evaporation of contaminants on graphene lattice while the temperature reaches up to 2000 K and beyond depending on device geometry. In the case of a heterostructure, at a bias of 3 V over the suspended sample, we observed the gradual transformation of 2D MoS2into 3D nanocrystals followed by processes such as vacancy formation, void expansion and edge evaporation.

In summary, this work explored the different methods to structurally modify the multidimensional heterostructures (1D/2D and 2D/2D) and could be extended to entire range of low-dimensional materials and their stack combinations to get insights into growth, dynamics and evolution of materials and establish new nanofabrication technique.