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Review article

Spatially-resolved studies on the role of defects and boundaries in electronic behavior of 2D materials

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ABSTRACT

Two-dimensional (2D) materials are intrinsically heterogeneous. Both localized defects, such as vacancies and dopants, and mesoscopic boundaries, such as surfaces and interfaces, give rise to compositional or structural heterogeneities. The presence of defects and boundaries can break lattice symmetry, modify the energy landscape, and create quantum confinement, leading to fascinating electronic properties different from the "ideal" 2D sheets. This review summarizes recent progress in understanding the roles of defects and boundaries in electronic, magnetic, thermoelectric, and transport properties of 2D layered materials. The focus is on the understanding of correlation of atomic-scale structural information with electronic functions by interrogating heterogeneities individually. The materials concerned are graphene, transition metal dichalcogenides (TMDs), hexagonal boron nitride (hBN), and topological insulators (TIs). The experimental investigations benefit from new methodologies and techniques in scanning tunneling microscopy (STM), including spin-polarized STM, scanning tunneling potentiometry (STP), scanning tunneling thermopower microscopy, and multi-probe STM. The experimental effort is complemented by the computational and theoretical approaches, capable of discriminating between closely competing states and achieving the length scales necessary to bridge across features such as local defects and complex heterostructures. The goal is to provide a general view of current understanding and challenges in studying the heterogeneities in 2D materials and to evaluate the potential of controlling and exploiting these heterogeneities for novel functionalities and electron devices.

Abbreviations: 0D, zero-dimensional; 1D, one dimensional; 2D, two-dimensional; 3D, three-dimensional; AFM, atomic force microscope; BL, bilayer; CVD, chemical vapor deposition; DFT, density functional theory; dI/dV, differential tunneling conductance; DOS, density of states; EBID, electron beam induced deposition; E_D, dirac point; E_F, Fermi energy; GB, grain boundary; hBN, hexagonal boron nitride; LEEM, low-energy electron microscopy; MIM, microwave impedance microscopy; ML, monolayer; QHE, quantum hall effect; SEM, scanning electron microscope; SPM, scanning probe microscopy; SQUID, Superconducting Quantum Interference Device; STM, scanning tunneling microscopy; STP, scanning tunneling potentiometry; STS, scanning tunneling spectroscopy; TI, topological insulator; TL, trilayer; TMD, transition metal dichalcogenides; TSS, topological surface states; UHV, ultra-high vacuum; VBM, valance band maximum; vdW, van der Waals; V_{th}, thermoelectric voltage; XPS, X-ray photoelectron spectroscopy; μ-LEED, micro low-energy electron diffraction.

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Contents

1. Introduction

Two-dimensional (2D) materials often contain atomic defects and mesoscopic boundaries. The physical origin for these imperfections is thermodynamic laws that favor fluctuation and disorder over long-range order in low dimensional systems [1,2]. The defects and boundaries can break transitional or rotational lattice symmetry, modify energy landscape, and create quantum confinement. It is these heterogeneities that often dictate the electronic properties of 2D materials, particularly the electron scattering, transport, and excitation processes. Thus the research on 2D materials must go beyond "ideal" or structurally averaged systems to consider heterogeneities. Understanding the roles of heterogeneities in 2D represents a grand challenge to materials research and offers a transformative opportunity to control electronic properties and energy-relevant functionalities.

The broad family of 2D materials offers great choices to the study of defects and boundaries and their effects on a variety of electronic behaviors [3]. Besides graphene, transition metal dichalcogenides (TMDs), hexagonal boron nitride (hBN), and 2D layers of pure elements, such as phosphorus or boron, can complement or even surpass the properties of graphene in

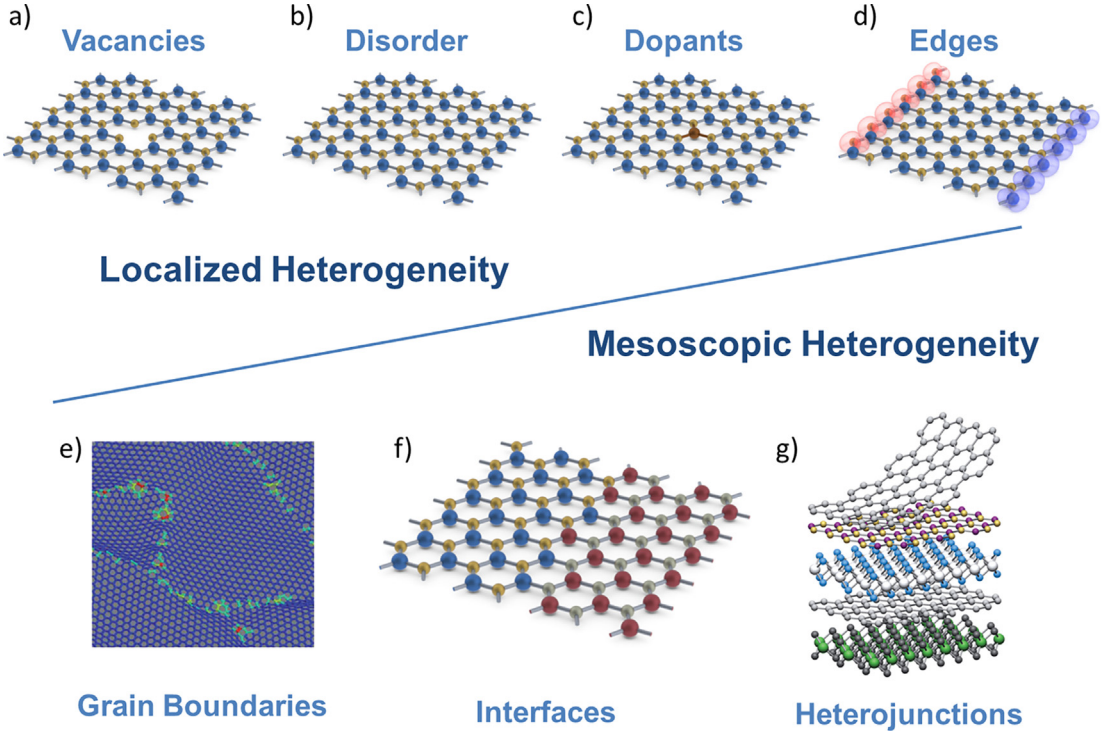

Fig. 1. Heterogeneities in 2D Materials. In 2D materials, (a–d) vacancies, disorder, dopants and edges create localized heterogeneities. Mesoscopic heterogeneities include (e–g) grain boundaries, interfaces and heterojunctions. Adapted with permission from (e) reference [175] Copyright 2013 The Royal Society of Chemistry, (g) from reference [123], Copyright (2013) Nature Publishing Group.

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