

Defects in semiconductors

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I. INTRODUCTION

Defects are crucial to understanding semiconductor materials and designing semiconductor-based devices. In using the term “defects,” we include not only native point defects (such as vacancies and interstitials), but also dopant impurities, unintentional contaminants, and complexes between these species. While some defects can lead to detrimental nonradiative recombination and carrier trapping, other defects can be used to provide free carriers that are necessary for the design of transistors, light-emitting devices, and solar cells. Since the advent of semiconductors, a significant amount of research has focused on how to deduce and control the behavior of these defects. While traditional materials (such as silicon, germanium, and gallium arsenide) continue to present challenges in terms of understanding defects, a surge of interest in power electronics has motivated the study of newer classes of materials such as two-dimensional semiconductors and wide-bandgap nitrides and oxides. Growing interest in this area has sustained the relevance of longstanding international conferences such as the International Conference on Defects in Semiconductors.¹

As sources of electrical, optical, magnetic, and vibrational signals, defects in semiconductors provide an excellent testing ground for both theory and experiment. This Special Topic brings together contributions from researchers with wide-ranging expertise in the field of defects in semiconductors, documenting advances in our understanding of established materials like silicon carbide and gallium arsenide, but also includes progress in promising new materials, such as the II-IV-VI ternary compounds and ultrawide-bandgap oxides. While showcasing the latest breakthroughs in defects in semiconductors, we also wish to acknowledge the passing of our dear colleagues Audrius Alkauskas² and Władysław Walukiewicz,³ both of whom made fundamental contributions to this field.

II. BACKGROUND

As discussed above, defects in semiconductors can be native (or intrinsic), involving only those elements that compose the bulk compound. The introduction of extrinsic impurity elements, necessary for doping, also leads to the formation of defect species. Categorizing defects as intrinsic or extrinsic is often helpful for categorizing their behavior; sorting defects by dimensionality is often helpful as well. Most of the defects discussed in this Special Topic are “zero-dimensional” point defects, as they involve a defect on a single (or in some cases, a few) lattice sites. Defects can also have higher dimensionality: “one-dimensional” defects include dislocations, and stacking faults can be thought of as “two-dimensional defects,” both of which are also often crucial for understanding semiconductor behavior.

In this Special Topic, we categorize defects not by their chemical nature or dimensionality but instead by their semiconductor host material. Our hope is that this will allow the reader to quickly find the material classes of interest. Nevertheless, examining defect behavior across different materials systems is quite useful for understanding their underlying physics. While a fuller discussion of defect physics is beyond the scope of this Editorial, recent works^{4–6} provide much greater detail.

III. SUMMARY OF RESEARCH AREAS

A. Methodological advances in defect modeling and experimentation

The challenge of studying defects necessitates constant improvements and new developments in methods, both in theory and experimentation. Several of the works published in this issue describe such advancements.

Many of the papers in this area were motivated by the need to understand the role of defects in electronic devices. While defects

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