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Defects in semiconductors FREE

Special Collection: Defects in Semiconductors 2024

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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 Alkauskas[2] and Wladyslaw 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

are often detrimental to device performance, it has been shown that the capture and emission of carriers from defect levels can actually be utilized to make resistive switches. In Ref. 7, the authors develop an analytical model of the defect trapping/detrapping processes in the operation of such devices, and demonstrate how it can be used for device operation and design. Reference 8 explores how intentionally adding a defective layer to silicon-on-insulator device structures can benefit electronic devices for radio frequency applications. The study develops and validates a simulation methodology to model the influence of defects on increasing the resistivity for higher harmonics of a coplanar waveguide structure and provides insight for designing the defective layers.

Machine learning (ML) has proved to be promising for finding subtle patterns in complex data. In Ref. 9, the authors demonstrated that ML can be used to interpret Raman spectra to categorize the amount of radiation damage present in the sample. This opens the door for Raman to be used as a nondestructive method for characterizing defects in electronic devices.

Also, specialized methods are required to deal with the unique aspects of defects for quantum devices and quantum materials. While the negative charge state of the NV center in diamond (NV^-) is the prototypical defect for quantum applications, the properties of the neutral charge state (NV^0) are essential for the photoionization processes of NV^-. Also, NV^0 has been suggested as a quantum defect in its own right. In Ref. 10, the authors use DFT methods to tackle the complicated electronic structure of NV^0, including its optical and spin properties, as well as pathways for ionization to and from NV^-. A key aspect of quantum defects is how they couple with their environment, including other defects/dopants and nearby surfaces. Such interactions can reduce coherence times, or act as a handle for engineering defect properties and defect–defect interactions. Reference 11 develops a model indicating how to initialize shallow NV^- centers via a charge-transfer mechanism enabled by the NV's charge-state-dependent electroluminescence. The role that defects play in influencing the properties of materials depends on the electronic structure of the host. Topological semimetals are a unique class of materials defined by an electronic structure involving linear band touchings near the Fermi level. In Ref. 12, the properties of defects in such materials are reviewed, including theoretical and experimental approaches for studying defects in these materials, and unique challenges and opportunities associated with defect engineering.

Several of the papers address technical aspects of computational calculations based on density functional theory (DFT). One of the critical issues with modeling defects using DFT is the accurate treatment of localized states, which can be hindered by self-interaction errors. In Ref. 13, the authors investigate the approach of using nonempirical semilocal density functionals, corrected via an additional weak local potential, for correcting the self-interaction of polaronic states.

Though much of the formalism surrounding DFT calculations for basic properties of point defects is somewhat established, defect calculations are methodologically complex, requiring several distinct steps to process the computational data into physically accurate results. The goal of Ref. 14 is to develop tools to automate this procedure so that defect calculations can be performed in a high-throughput fashion without sacrificing their quality. This is crucial for exploring the staggering design space that defects represent. Often, theoretical studies of defects operate under the simplifying assumption of thermodynamic equilibrium. However, kinetic processes involving defects, specifically defect diffusion, play a crucial role in the distribution of defects in any material during growth or processing. Theoretical models of defect diffusion are reviewed in Ref. 15, and first-principles methods are utilized to make quantitative comparisons with experimental observations of diffusion profiles in several wide-bandgap semiconductors.

Another challenge of DFT-based defect calculations is how to systematically assess uncertainty in the calculated parameters. This issue is tackled by the authors in Ref. 16, where Bayesian error estimation is applied to quantify uncertainty of defect formation energies determined via DFT.

Finally, as mentioned above, Ref. 2 discusses the seminal contributions to the computational study of defects by Audrius Alkauskas, who passed away in 2023. These include the theoretical description and methodological developments necessary to determine the coupling of defects to the crystal lattice relevant for carrier capture and recombination, the properties of quantum defects in semiconductors, and the physics of defects in two-dimensional materials.

B. Defects in oxides

1. Defects in gallium oxide and related materials

Wide-bandgap oxides continue to enthrall the community studying defects in semiconductors. In particular, gallium oxide (Ga_2O_3) has attracted significant attention for its potential use in power electronics. Islam *et al.* have studied[17] phonon-induced Urbach tails in doped β-Ga_2O_3 to understand their role in electrical breakdown. Planar defects are also of interest, as Myasoedov *et al.* have used transmission electron microscopy to study[18] their behavior in α-Ga_2O_3 grown by hydride vapor-phase epitaxy.

Interfaces and heterostructures involving Ga_2O_3 are also a notable research topic. Takane *et al.* have reported structural characterizations of dislocations in α-Ga_2O_3 thin films on *c*- and *m*-plane sapphire substrates.[19] Aafiya *et al.* have probed the electronic and dielectric properties of stacked layers of Ga_2O_3 and Al_2O_3 synthesized via atomic layer deposition.[20] Also, using atomic layer deposition to grow ZrO_2/β-Ga_2O_3 capacitors, Chen *et al.* have investigated interface states and bulk traps.[21] Employing theoretical calculations, Hattori *et al.* studied how GaO_x interfacial layers affect the properties of the GaN/SiO_2 interface.[22]

The role of native point defects is among the most pressing in the study of gallium oxide. Measuring temperature-dependent capture cross sections, Vasilev *et al.* examined[23] the character of deep-level defects in β-Ga_2O_3. Ga vacancy defects are specifically probed in a study of as-grown and irradiated β-Ga_2O_3 that uses positron annihilation spectroscopy.[24] Stavola *et al.* also provide a Tutorial[25] on the infrared detection and calculation of O–H centers in β-Ga_2O_3.

Finally, research on the behavior of impurity dopants in Ga_2O_3 is another major topic of study. Using optical and electrical characterization, Remple *et al.* investigate the effects of electron irradiation on Hf- and Zn-doped material.[26] Employing deep-level transient spectroscopy (DLTS), Dawe *et al.* characterize deep-level

traps in β-Ga_2O_3 epilayers.[27] With both DLTS and DFT, Langørgen *et al.* describe the identification of electrically active defects and dopants in β-Ga_2O_3.[28] Also using DFT, Seacat and Peelaers determine how $(In_xAl_{1-x})_2O_3$ alloys can be doped *n* type.[29]

2. Defects in other oxides

Though Ga_2O_3 has been a center of attention, many other oxides remain of great interest. These include zinc oxide, as Mandal *et al.* report on how oxygen vacancies affect the luminescent properties of Dy-doped ZnO.[30] Venzie *et al.* discuss the kinetics of H diffusion in SnO_2, which they study using vibrational spectroscopy.[31] From both theory and experiment, Fowler *et al.* provide a Perspective[32] on the metastability of cation vacancy structures in a set of semiconducting oxides. Other oxides being studied include $SrTiO_3$, as Kumar *et al.* report on the effect of ion implantation on the electronic structure of this material based on x-ray diffraction and photoemission measurements.[33]

Achieving *p*-type conductivity in wide-gap oxides continues to attract interest. In the case of $LiGa_5O_8$, Lyons reported the behavior of deep, polaronic acceptors.[34] Ananchuensook *et al.* explore how hydrogen passivation of acceptor dopants can enhance *p*-type conductivity in copper delafossites.[35] Using thermally stimulated current measurement techniques, Isik *et al.* address defect centers in $PbWO_4$ single crystals.[36] Finally, Xu *et al.* present results on a $Ag@SnO_2/CsPbBr_3$ nanocomposite gas sensor that operates at room temperature.[37]

C. Defects in III-Vs

III-V semiconductors, such as gallium arsenide (GaAs) or aluminum nitride (AlN), have long been the subject of defect-related work. Issues still persist for well-studied materials (e.g., GaAs), and newer materials like the II-IV-V compounds (such as $ZnGeP_2$), provide test cases for existing theories of defect behavior.

1. Gallium arsenide

Chakravorty *et al.* use synchrotron-based high-resolution x-ray diffraction to analyze GaAs and 4H-SiC irradiated with Ar and Ag ions, and highlight the complex interplay between displacement damage and ionization energy loss.[38] In Ref. 39, Barthel *et al.* examine how doping concentration degrades the performance of GaAs solar cells through trap-assisted tunneling and damage induced by different types of radiation. Finally, Yu *et al.* examine the prospects for using pulsed laser melting as a means to overcome the doping limits posed by compensating defects in GaAs.[40]

2. Gallium nitride

In Refs. 41 and 42, Vorobiov *et al.* and Reshchikov *et al.* analyze photoluminescence in GaN doped with Mg, Be, Ca, Cd, and Hg, where they identify distinct emission bands associated with each of these impurities. The authors corroborate these results using first-principles calculations based on hybrid functionals. Also using first-principles calculations, Lee *et al.* explore native point defects and unintentional impurities in $Al_{1-x}Gd_xN$, finding that nitrogen vacancies are likely the most prevalent native point defect in these rare-earth nitride alloys.[43]

Sun *et al.* combine a wide range of experimental techniques, including deep-level transient spectroscopy (DLTS), photoluminescence and electrical transport measurements, to investigate the properties of Fe in AlGaN alloys. They show that the presence of Fe in AlGaN can lead to the degradation of performance of AlGaN devices.[44] Finally, Loeto *et al.* use cathodoluminescence measurements to assess the damage caused in GaN due to focused ion beam processes that rely on Ga or Xe ions.[45] The authors find a lower degree of damage when using Xe compared to Ga ions.

3. II-IV-V compounds

Gustafson *et al.* use electron paramagnetic resonance measurements to investigate the properties of Se-doped $ZnGeP_2$ and present evidence for the neutral charge state of the Se donor.[46] Using first-principles calculations of point defects in $ZnGe(P,As)_2$ Wang *et al.* also draw attention to the role of anion–cation antisite pair defects which they find have low formation energies in this class of materials.[47]

D. Defects in silicon carbide

Identifying the different experimental conditions that lead to the incorporation of point defects and extended defects in the different polymorphs (e.g., 4H, 6H) of SiC remains an active area of research and relies on a range of experimental techniques such as photoluminescence, DLTS, and transmission electron microscopy. Alfieri *et al.*, Ousdal *et al.*, Kumar *et al.* Yang *et al.*, and Ishiji *et al.* use some of these measurement approaches to identify extended defects[48] and point defects in SiC due to proton irradiation,[49,50] thermal oxidation,[51] and formation of electrical contacts.[52] These experimental findings can be compared to predictions from first-principles calculations such as those reported by Huang *et al.* and Smith *et al.* on candidate point defects in 4H-SiC.[53–55]

E. Defects in 2D materials

Defects in two-dimensional (2D) semiconductors are also a topic of great interest, including in well-studied materials like the transition metal dichalcogenides, and also novel materials such as silicene. Using resonant Raman spectroscopy, Tariq *et al.* studied non-stoichiometry due to chalcogenide vacancies in $MoSe_{1.8}S_{0.2}$ single crystals.[56] Anvari *et al.* compute the effects of native point defects on the electrical behavior of MoS_2 and MoS_2/Au(111) heterojunctions.[57] Finally, Raji *et al.* perform a DFT study of vanadium dopants in monolayer silicine.[58]

F. Defects in detector/absorber materials

Alloying of ternary or quaternary semiconductors offers spectral tunability, but often introduces difficulties in decoding the behavior of defects. Chen *et al.* have used first-principles calculations to identify deep levels associated with native defects in HgCdTe,[59] an important detector material. In Ref. 60, Gutmann *et al.* use diffuse scattering experiments together with Monte Carlo simulations to understand relaxations around defects in CdZnTe. Also combining experiment and DFT calculations, Vilão *et al.* investigate[61] muonium/hydrogen states formed in $Cu(In,Ga)Se_2$ and Cu_2ZnSnS_4.

G. Defects in silicon

Finally, a number of issues still exist surrounding the behavior of defects in silicon, the quintessential semiconductor, and related materials systems. For instance, Becker *et al.* have investigated misfit dislocation glide in $Si_{1-x}Ge_x$/Si(001).[62] Nikolskaya *et al.* also report on stable, optically active defects emitting at 1240 nm in irradiated SiO_2/Si.[63] In a two-part experimental[64] and theoretical[65] study, the behavior of defects during the growth of highly P-doped Si is discussed, in order to understand the interaction of dopants with dislocations and stacking faults.

IV. CONCLUSIONS

The investigation of the behavior of defects in semiconductors, using both theoretical and experimental approaches, remains vigorous. Important issues still remain, not only in the study of mature materials such as silicon, but also in emerging materials such as wide-bandgap oxides. This Special Topic on "Defects in Semiconductors" provides a snapshot of those issues that continue to intrigue our research community. We believe that the fundamental study of defects in semiconductors, like those included in this Special Topic, will provide insights valuable for a number of fields, including quantum information science, power electronics, and energy storage and conversion.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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