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Defects in semiconductors

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I. INTRODUCTION

Defects create key functionalities in semiconductor devices by contributing with charge carriers or assisting optical transitions. On the other hand, defects may cause severe degradations in the device performance, e.g., by enhancing unwanted carrier recombination. Understanding defects has been a continuous endeavor in traditional semiconductors, such as silicon (Si) and gallium arsenide, and is critical in the development of new semiconductors and components. Thus, defects in semiconductors remain a vibrant field of research, as highlighted by the increasing attendance of the relevant international conferences, such as the International Conference on Defects in Semiconductors.[1]

The research field of defects in semiconductors encompasses a wide range of topics, combining theoretical modeling and experimental investigations. Central to the field is the pursuit for a fundamental understanding of point and extended defects, including electrical, vibrational, optical, and magnetic phenomena; this is essential for mastering emerging materials, such as wide-bandgap semiconductors, doped nanoparticles, and 2D materials as well as in well-established material systems. Indeed, substantial advances have been reported during the last few years. For example, in silicon (Si), much attention has been devoted to understanding of the degradation mechanisms, specifically that of the light induced degradation (LID) as well as the light and temperature induced degradation (LeTID). In silicon carbide (SiC), understanding the lifetime-limiting defects is still of utmost importance for power electronic devices. In nitrides, studies of the defects related to the light emission control remain an important endeavor. In less developed material systems, such as gallium oxide (Ga_2O_3) and other oxides, compensating defects and defects influencing the charge carrier concentration are intensely studied, and this applies also to perovskites and other emerging materials for thin-film technologies.

Dimensionality has become an important topic too, with nanostructures, and more recently 2D materials, approached a level of quality needed for advanced defect studies. Another field that is booming and expected to grow even more in the coming years is defects related to quantum technology (QT). Indeed, point defects in semiconductors as a platform for quantum technology have received tremendous attention not only for qubits in quantum computers, but also for a wide range of applications within quantum communication, computing, and sensing. Over the last few years, the field of point defect based QT has increased dramatically since properties similar to those of the well-established nitrogen-vacancy (NV) center in diamond were demonstrated in a more industrially friendly platform of SiC and Si.

Hand in hand with the advancement of understanding defects in semiconductors goes the development of theoretical and experimental tools. Importantly, the number of studies that combines the theoretical and experimental approaches increased, improving the methodology. The present collection taps in on the current temperature samples the current state in the field. The present collection of articles represents the current understanding of the different material systems, and as exemplified above, it envelopes important trends in the field.

II. BACKGROUND

Semiconductor defects can be categorized in a variety of ways. One may, for example, consider the dimensionality, where point defects are the imperfections that occur at specific locations, of the crystal, and often considered zero dimensional. Point defects in crystals can be intrinsic, also called native defects, which involve only the host crystal atoms, or can be of extrinsic nature involving impurity atoms. When an impurity is deliberately introduced into a semiconductor to alter the electrical properties, it is referred to as a dopant. A defect can occupy a substitutional or interstitial lattice site. A vacancy or a matrix atom in an irregular interstitial position (self-interstitial) is an example of native defects. Notably, vacancies and self-interstitials may be created when an energetic particle, such as a proton, knocks out atoms of the lattice sites.

In contrast, in "1D" defects, such as dislocations, where an extra plane of atoms is in the lattice, the edge of that plane is a line and is referred to as an edge dislocation. More complicated defect types include stacking faults, where a plane of atoms is in a wrong sequence and can be seen as a 2D defect. All these defects may be present in a significant concentration, even in relatively mature materials, and severely affect the properties. More detailed information about semiconductor defects, growth, and characterization of semiconductors can be found in, e.g., Refs. 2 and 3.

III. SUMMARY OF AREAS COVERED

A. Defects in group IV semiconductors

Semiconductors from group IV of the periodic table, such as Si and SiC, are mature materials with decades of development, including defect studies. Still, this is a very active field of research, motivated by advances in the conventional electronics industry, power electronics, solar cells as well as quantum technology. For example, understanding recombination and degradation mechanisms is important for solar cells, and the "Defects in Semiconductors" Special Topic discuss electrical and theoretical results related to the interaction between boron, gallium, indium, and aluminum with the oxygen dimers.[4] On the process side, the behavior of oxygen precipitates in Si wafers after rapid thermal processing (RTP) at 1350°C in an oxygen atmosphere was monitored by infrared (IR) tomography.[5] Iron is an important impurity both in solar cell technology and a silicon-based integrated circuit. The ultrasound impact on iron–boron pair transformation and dissociation has been shown by measuring short circuit current kinetics.[6]

Ion-irradiation may induce deformation of free-standing ultrathin Si wafers, as revealed by the time-response spectrum, upon deformation as measured using a laser displacement meter. It was found that fast deformation originated from expansion or shrinkage of the crystal lattice was caused by beam heating. It was concluded that the deformation rate depends on the topological defect formation in Si crystals; in particular, the slow deformation is related to the coordination number of disappeared topological defects.[7] The nature of radiation-produced defects in strongly doped p-type silicon that are stable at room temperature reveals two types of dominant boron-related complexes, which are attributed to the substitutional boron-interstitial boron pair (being neutral in p-type Si) and the substitutional boron–divacancy complex (displaying donor activity).[8] The Special Topic also includes experimental and theoretical explorations of the low-frequency electrically detected magnetic resonance (EDMR) response from spin-dependent trap-assisted tunneling on unpassivated $^{28}Si/^{28}SiO_2$ metal–insulator–semiconductor (MIS) capacitors.[9]

In SiC, several intrinsic and important defects remain to be identified experimentally and understood. An example of such is the M-center, which has recently been tentatively identified as the carbon interstitial.[10] Carbon interstitials have remained elusive in SiC but play a key role in the suppression of the lifetime killing defect—the carbon vacancy. At the same time, the conventional carbon cap used during heat treatments acts as a source of carbon interstitials. Carbon interstitials have now been observed during heat treatment with a carbon cap and do not only result in the M-center, but also other defect levels in the same range.[11] Investigations of compensation of native defects and self-compensation in Al-doped 4H-SiC reveal that the positively charged carbon vacancies (V_C^{2+}) are also the dominant compensating centers in Al-doped 4H-SiC.[12] In the Perspective by Bathen *et al.*,[13] some of the main defect characterization techniques are reviewed for the development of SiC technology.

B. Defects for quantum technology

The prospects of using defects in quantum technology have spurred massive research efforts in recent years. The "Defects in Semiconductors" Special Topic encompasses both perspectives and recent results within this exciting field of research. In addition to the well-known nitrogen-vacancy (NV) center in diamond, silicon carbide color centers integrated into photonic devices span a wide range of applications in quantum information processing in a material platform with quantum-grade wafer availability and advanced processing capabilities. Reference 14 gives a perspective on conceptual and quantitative analysis of the role of silicon carbide integrated photonics in three key application areas: quantum networking, simulation, and computing. Further perspectives on widefield microscopy to produce spatially resolved maps of local quantities, such as magnetic field, electric field, and lattice strain, are discussed in Ref. 15. Zwier *et al.* investigated the implementation of electromagnetically induced transparency (EIT) with c-axis divacancy color centers in silicon carbide. Indeed, EIT can be established with high visibility also in this material platform upon careful design of the measurement geometry.[16] The Special Topic also contains a study of the differences that arise in quantum dots with respect to process-induced defect densities, and inhomogeneous strain is reported by Stein *et al.*, where it is shown how to minimize the interface trap density by annealing.[17]

Integrated optics becomes important for enhancing and controlling quantum compatible defects acting as single photon sources, but the fabrication may result in considerable sample roughening, strain, and defect introduction. In this respect, testing novel methods for fabricating monolithic single-crystal integrated-photonic devices in SiC may further develop this area.[18] The fluorescence spectra of divacancies in SiC created by neutron irradiation in porous cubic SiC and nanoparticles formed by the no-photon exciton generation chemistry technique are analyzed in detail by means of first principles calculations.[19] They find that irradiation produces a larger shift in the fluorescence spectrum with residual background fluorescence. Importantly, aligned defects can be found or artificially designed in, e.g., transition metal dichalcogenides. Han *et al.* have investigated the mechanical behavior of single layer MoS_2 sheets with aligned defects under uniaxial tension by numerical calculation and theoretical modeling.[20]

C. Defects in oxide semiconductors

The wide bandgap and correspondingly a high breakdown field have made gallium oxide a promising material for power electronics and UV optoelectronics, which has led to strong research interest in recent years. The defect physics of Ga_2O_3 is particularly fascinating and important due to the low symmetry of the most stable phase, i.e., the monoclinic beta-phase. In the Perspective of

Huang *et al.*, an overview of recent characterization works involving scanning transmission electron microscopy (STEM) and related techniques reveals a detailed structure of various point and extended defects in β-Ga_2O_3 and β-$Al_xGa_{(1-x)2}O_3$ heterostructures to gain an atomic level understanding of the structure of the defects and how they correlate with important properties.[21] Hole polarons are expected to be of utmost importance in wide- and ultra-wide bandgap oxides, including gallium oxide, and hampers the ability for p-type activity. This is a general feature for several of the ultra-wide bandgap materials, as shown using theoretical calculations.[22] The formation of small polarons is also important in other oxides, for example, in hematite (Fe_2O_3), as calculated by Smart *et al.*[23]

Hydrogen plays an important role in Ga_2O_3 as it is electrically active and an omnipresent impurity. Several O–H and O–D vibrational lines for complexes that involve impurities that are shallow donors and deep acceptors have been reported recently. Vibrational properties of complexes that involve shallow donors (OD–Si and OD–Ge) with complexes that involve deep acceptors (OD–Fe and OD–Mg) can be revealed by Fourier transform infrared spectroscopy (FTIR).[24] Hydrogen is electrically active and may form defect levels in the bandgap, as revealed by deep level transient spectroscopy. Indeed, the defect level previously labeled E1 in DLTS studies is proposed to be originating from an H-related defect complex, where hydrogen on an oxygen site, a divacancy complex with one hydrogen, and a donor complex with hydrogen are proposed as potential candidates for this level.[25] Iridium is used in the crucible during the growth of Ga_2O_3 and is incorporated and acts as a deep donor. It can act in several defect reactions and can be observed by, e.g., electronic Raman scattering.[26] Smirnov *et al.* report on comparison between theoretical calculations and experimental data on the critical film thickness of a α-$Ga_2O_3$$\alpha$-$Al_2O_3$ heterostructure. In particular, the effect of Al composition (x) and the growth direction on the critical film thickness for misfit dislocation formation in α-$(Al_xGa_{1-x)2}O_3/\alpha$-$Al_2O_3$ heterostructures have been studied.[27] Implantation induced structural transformation has recently been observed in Ga_2O_3.[28,29] In Ref. 30, the defect accumulation and annealing phenomena are observed after implantation, and subsequent annealing in layers transformed by Si implantation is studied using Rutherford backscattering spectrometry (RBS), x-ray diffraction and STEM, and where the structural transformation back to the beta-phase is highly fluence dependent.

Obviously, other oxides are also of high scientific and technological importance. The "Defects in Semiconductors" Special Topic includes theoretical calculations of the formation of oxygen vacancies (VO) in strained Ti-based oxides that reveal an almost linear dependence on the changes in the cell volume, bandgap, and Ti–O bond strength of the host oxide.[31] Fourier transform infrared spectroscopy (FTIR) combined with theoretical calculations are used to reveal hydrogen-related defects in natural anastase TiO_2.[32,33] Barium titanate samples exhibiting persistent photoconductivity display a broad infrared (IR) absorption peak at 5000 cm^{-1} (2 μm), attributed to polaronic or free-carrier absorption.[34] A model is proposed to precisely estimate the density of dislocations in ZnO using the full width at half maximum (FWHM) of omega-scans.[35] Subgap trap density of states (DoS) has been measured by ultrabroadband photoconduction to study hydrogen incorporation into the channel layer of top-gate amorphous indium gallium zinc oxide (a-IGZO) thin-film transistors (TFTs).[36] The low electronic conductivity of hematite (α-Fe_2O_3) is a hindrance for its utilization in a range of applications. In Ref. 37, density functional theory with thermodynamic analysis is explored to compute the concentration of electronic defects in hematite as a function of the oxygen partial pressure.

D. Defects in nitrides

The family of nitride based semiconductors can be considered mature materials, but there is still an active field of research and, in fact, has seen an increased attention in the last few years. One of the dominant defect types in GaN is basal plane stacking faults. They can be studied using scanning electron microscopy that combines the structural characterization by electron channeling contrast imaging with the optical characterization by cathodoluminescence hyperspectral imaging.[38] A correlation between a fine dislocation core structure and the luminescence bands at 3.1, 3.2, 3.3, and 3.35 eV is established by careful microindentation of an a-plane free-standing semi-insulating Fe-doped GaN sample.[39]

The so-called yellow luminescence (YL) and orange luminescence (OL) photoluminescence lines in GaN have been investigated extensively, including their evolution upon thermal annealing. In Ref. 40, a combination of PL and density functional calculations is utilized, where the YL2 band with a maximum at 2.3 eV observed by PL appears to be related to the VGa–3Hi complex. After thermal treatments above 600°C, the YL2 band is replaced by two new PL bands: the OL3 band with a maximum at 2.1 eV and the RL4 band with a maximum at 1.6–1.7 eV. Be incorporation on the gallium site (Be_{Ga}) was studied using photoluminescence after Be implantation and subsequent annealing. It was found that the ultraviolet luminescence band with a maximum at 3.38 eV attributed to the shallow Be_{Ga} acceptor appeared only in implanted samples with high temperature anneals and ultrahigh N_2 pressure.[41]

Eu doping is one approach to tune the color from red to orange to yellow in GaN based devices operating as LEDs. Defects play a crucial role in the mechanism for light emission that has been modeled to determine the optimal injection conditions to maximize the gamut of color tunability while minimizing power consumption.[42] Terbium-doped semiconductors are candidates for novel full-color light sources in next-generation displays. The luminescence properties of $Al_xGa_{1-x}N$:Tb are studied, and the luminescence is clearly observed at room temperature.[43] Surface and interface states can be investigated using x-ray photoelectron spectroscopy, and in Ref. 44, it was shown that plasma-based dry etching methods may inhibit the internal screening of this bound charge and, thus, increase the concentration of externally charged states. In Ref. 45, threading dislocations and point defects were observed in $Al_{0.9}Ga_{0.1}N$/GaN heterostructures, and a link between the mobility and the quality of interfaces is established. Formation of wurtzite phase inclusions may occur in zincblende GaN epilayers. High-resolution transmission electron microscopy along with four-dimensional STEM reveals the origin of the wurtzite inclusions in the nucleation layer and at the GaN/AlGaN interface.[46] Defects formed during epitaxial growth and regrowth have

been characterized using scanning Kelvin probe force microscopy and scanning capacitance microscopy in Ref. 47. Yu *et al.*[48] explore the leakage current mechanism in ion implantation isolation (I/I/I) regions of GaN high electron mobility transistors.

E. Defects in thin-film semiconductors

Defect tolerance has been highlighted as essential to the impressive photovoltaic performance of halide perovskites. This defect tolerance concept is critically analyzed in the recent Perspective by Zhang *et al.*[49] In fact, density functional calculations indicate that the nonradiative recombination rates in halide perovskites are comparable to or even greater than those in more conventional semiconductors. Similar to the case of conventional semiconductors, defect engineering is still key to improving the efficiency of perovskite solar cells. The Special Topic also contains a perspective on structural and dynamical disorders in halide perovskites used in applications from energy harvesting to high brilliance incoherent and coherent light emitters.[50] The $Pb(Bi_{1-x}Sb_x)_2(Te_{1-y}Se_y)_4$ topological insulator crystals reveal that the magnetoresistance agrees well with a three-dimensional weak antilocalization or weak localization model in the low temperature region below 20 K.[51]

IV. CONCLUSIONS

Experimental and theoretical studies of defects in semiconductors were made, and they continue to make major impacts on advancing electronic materials, enhancing energy efficiency in solid state devices, creating future quantum technology platforms, etc. Fundamental studies and functionalization of defects are a field of both a long tradition and a great potential for scientific and technological renewals. We trust that the present collection of papers in the "Defects in Semiconductors" Special Topic will be an important milestone for the community.

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