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Defects in Semiconductors

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I. INTRODUCTION

All semiconductors, whether by design or by accident, contain defects. The fundamental properties of defects, such as impurities, native defects, and extended defects, affect a broad range of applications. These technologically important defects may be introduced during growth and processing. Electrical, optical, and magnetic phenomena related to defects have been observed experimentally and studied theoretically in a variety of materials. In addition to traditional semiconductors (elemental, III–V, and II–VI), emerging materials include organic semiconductors, nitrides, oxides, and topological insulators, in bulk crystal and thin-film forms as well as low-dimensional and nanoscale structures.

Recent developments have highlighted the importance of understanding defects at a fundamental level. The efficiency of light-emitting diodes and solar cells, in particular those using novel materials, can be enhanced by controlling defect populations. Dopant spins and optically active centers are potential building blocks for quantum computers. III-nitrides continue to get a lot of attention, while complex oxides and gallium oxide are rising in popularity. Advances in thin-film growth, microscopy, spectroscopy, theory, and computational modeling are leading to an unprecedented glimpse into atomic-level properties of point and line defects. The dramatic increase in knowledge gained by these studies is enabling engineers to incorporate new functionalities into semiconductor devices.

II. BACKGROUND

Information about semiconductor defects, growth, and characterization of semiconductors can be found in Ref. 1, and more details about defect characterization are in a volume edited by Tuomisto.[2]

A *point defect* is an imperfection that occurs at a specific location, or point, in a crystal. This is in contrast to an *extended defect*, which is not confined to a specific lattice site. A *dislocation*, for example, is a one-dimensional "line" defect. When there is an extra plane of atoms in the lattice, the edge of that plane is a line and is referred to as an edge dislocation. A *stacking fault*, where a plane of atoms is in the wrong sequence, is an example of a two-dimensional defect.

Point defects in crystals fall into two categories: (1) *native* defects, which involve only the atoms of the host crystal, and (2) *extrinsic* defects, which involve impurity atoms. When an impurity is deliberately introduced into a semiconductor, it is referred to as a *dopant*. A defect can occupy a substitutional or interstitial site. A *vacancy*, or missing atom, is a type of native defect. Vacancies and self-interstitials may be created when an energetic particle such as a proton knocks the atom out of its lattice site.

Defects can introduce electronic levels into the bandgap, affecting the performance of devices. A donor level is one where the center becomes positively charged when it gives up its electron. In *n*-type silicon, for example, phosphorus donates an electron to the conduction band. An acceptor level is negative when occupied by an electron. Mg acceptors in Ga_2O_3, for example, compensate donors and are negatively charged. If a donor (acceptor) level is close to the conduction-band minimum (valence-band maximum), it is a *shallow* level. The electronic wavefunction of a shallow level is delocalized. A deep level, in contrast, is far from the band extremum and has a localized wavefunction.

The "Defects in Semiconductors" Special Topic in *Journal of Applied Physics* presents a collection of papers that cover a broad range of materials, centered around the fundamental properties of defects. It covers topics on experimental and theoretical investigations of important point and line defects.

III. SUMMARY OF AREAS COVERED

A. Group-IV semiconductors

Semiconductors composed of group-IV elements (C, Si, and Ge) continue to be an active area of investigation. First-principles

calculations have shed new light on two "old" defects in silicon: vacancy-donor pairs (E centers)[3] and the four-Cu complex[4] that gives rise to a sharp photoluminescence (PL) peak in the near-IR. The lifetime of excited states of Bi donors was measured as a function of stress and found to be very sensitive to phonon modes.[5] Recent experiments uncovered electronic levels introduced by carbon–hydrogen pairs in silicon and dilute SiGe alloys,[6] exposure to neutrons during neutron transmutation doping,[7] and proton irradiation of SiGe alloys.[8]

Boron implantation is a preferred method for p-doping of silicon and modeling transport is continually improving.[9] The distribution of boron in nanostructured silicon was compared to that of bulk material.[10] Results on self-diffusion in silicon nanopillars[11] and boron diffusion in germanium[12] have also been reported. Antimony doping of germanium makes the material n-type and affects its bandgap absorption properties.[13]

Along with diamond, SiC is a promising material for quantum-computing applications, with point defects acting as qubits. Hydrogen affects the charge states of defects such as vacancies, important for such devices.[14] Muon implantation was performed to simulate the effect of isolated hydrogen in SiC.[15] As with silicon, defects at the SiC/SiO_2 interface affect the performance of metal-oxide field effect transistors (MOSFETs).[16] Deep levels[17] and diffusion[18] in SiC continue to be important, timely topics. Theoretical studies of carbon-based materials, namely, single-walled nanotubes[19] and 2D carbon nitride,[20] have shed new light on the role of defects.

B. Group III–V semiconductors

Regarding "conventional" III–V semiconductors, articles in the "Defects in Semiconductors" Special Topic highlight developments in the growth of InP on silicon substrates,[21] magnetic properties of Fe dopants in InSb,[22] and the optical and structural properties of GaAsBi quantum wells.[23] Narrow-gap semiconductors continue to be an important area with studies on dislocations in InSb[24] and the optical properties of InAsSb-based mid-IR emitters.[25]

Owing to their relevance to light-emitting devices, GaN-based materials are investigated intensively. The growth of GaN[26] and InGaN/GaN quantum-well structures[27] on silicon substrates results in extended defects such as V-pits and line defects. Deep levels were observed in an InGaN/GaN quantum well with an InAlN layer underneath.[28] Properties of dopants in GaN are important for a variety of applications. The implantation of Mg acceptors is a potentially beneficial way to achieve p-type conductivity but annealing remains a challenge.[29] The distribution,[30] magnetic properties,[31] and optical properties[32] of rare-earth dopants in GaN were investigated. The theory of carbon impurities provided insight into the defect as well as theoretical methodology.[33] PL bands, which provide an important fingerprint for defects, show large shifts with excitation intensity and temperature.[34] Finally, theoretical calculations of vacancies in 2D GaN have been performed.[35]

C. Group II–VI semiconductors

Defects in plastically deformed ZnSe crystals were observed with cathodoluminescence, electron backscattered diffraction, and micro-Raman spectroscopy.[36] ZnO remains a material of significant interest with new results on PL spectroscopy of group-V donors[37] and defects caused by ion implantation.[38] The migration of defects under the influence of an electric field was studied by cathodoluminescence (CL) spectroscopy.[39] Studies of other important dopants were conducted for hydrogen,[40] cobalt,[41] and Li–Al co-doping.[42]

D. Ga_2O_3

Gallium oxide is an emerging material with potential applications in power electronics. New insight into PL spectra was provided by calculations of self-trapped holes and acceptors.[43] Czochralski-grown Ga_2O_3 contains Ir impurities, which may form pairs with Mg or H.[44] Electron paramagnetic resonance and other techniques elucidated the energy levels and local structure for Ir, Fe, and Mg.[45,46] Doping with Co was shown experimentally and theoretically to lower the Fermi level.[47] Finally, the polarization dependence of a hydrogen vibrational mode provided a novel means for determining the dielectric axes in Ga_2O_3.[48] The role of disorder in amorphous oxides was studied for the case of In_2O_3.[49]

E. Ternary semiconductors

Combining three or more elements is a way to optimize properties such as lattice constant and bandgap for specific applications. Chalcopyrites, such as $Cu(In,Ga)Se_2$ (CIGS), are promising materials for thin-film photovoltaics. The effect of Cu and Ag vacancies in this materials system was investigated in Ref. 50. The properties of the Urbach tail, optical absorption that extends into the bandgap, were studied in ternary chalcopyrites.[51]

Complex oxides such as $SrTiO_3$ exhibit a range of electronic, magnetic, and optical phenomena. The oxygen vacancy concentration vs depth in $SrTiO_3$ was studied by CL,[52] providing insight into a defect that causes n-type conductivity in some (but not all) complex oxides. Theoretical calculations provide promising leads for a number of novel materials. Progress has been made on the theory of vacancies in TiNiSn,[53] acceptors in $ZnGeN_2$,[54] point defects in PbCdTe[55] and $LiGaO_2$,[56] and $ZnMoO_4$ surfaces.[57]

IV. CONCLUSIONS

Experimental and theoretical studies of defects in semiconductors have a major impact on energy efficiency, quantum computing, and many other applications. New materials are emerging and will require a fundamental knowledge of native and intrinsic defects. We hope the collection of papers in the "Defects in Semiconductors" Special Topic is enjoyed by the scientific community.

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