Program Overview

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Theory, Modeling and Simulation
Room Jefferson 1 & Atrium - Session TM-TuP
Theory, Modeling and Simulation Poster Session

TM-TuP-1 Simulation Study of Single Event Effects in Ga_2O_3 Schottky Diodes, ***Animesh Datta***, *U. Singisetti,* University at Buffalo

β-Ga_2O_3 has attracted high interest in the last decade and emerged as a promising material for next-generation power, GHz power switching, and RF applications. The large bandgap opens its possibilities for potential space applications, as the electron-hole pair generation in radiation (LET) is inversely proportional to the bandgap. Under radiation conditions in space, single event effects (SEE) are a potential reliability issue for devices in space-based RF and power systems. Previous reports have explored SEE burnout in SiC MOSFETs and thus SEE could also be an issue in Ga_2O_3 based devices. To date, there have been no reports of study of SEE in Ga_2O_3 based devices. In this work, we present the SEE effect in Ga_2O_3 Schottky diodes by simulation. 2-D simulations were performed using Silvaco TCAD to investigate the effects of ionizing radiation (measured in LET) under various bias conditions to understand the failure mechanism in the device. Breakdown simulations (V_{br}= 1400 V) show that the anode edge has the highest electric field; thus, it is chosen as the ion strike location in simulations. Under the radiation conditions, the time-dependent simulations show that the current recovers even at 1000 V and 40 MeV/mg/cm^2 LETs; even though the instantaneous peak field exceeds 8 MV/cm. It is noted that higher LETs take a longer time to recover. The heat generated due to ion strikes can also lead to the failure of devices due to thermal effects. The ion strike results in an instantaneous high current density within the device and leads to excessive Joule heating. The thermal effects were studied in Ga_2O_3 diodes with a diamond coating. Below radiation conditions of V=500V and LET=5 MeV/mg/cm^2 the device does not show any signatures of single event burnout (SEB) including thermal effects. At higher voltage bias and high LETs, there are signatures of possible thermal runaway where the temperature rises to a high value but only for a short amount of time and then recovers. The total energy dissipated under the ion strike condition is also calculated by integrating the power density spatially across the ion track. Our results indicate that under similar radiation conditions the power dissipated in b-Ga_2O_3 Schottky diodes is lower compared to the experimental data of SiC Schottky diodes. Future work includes investigating the threshold condition of SEB in b-Ga_2O_3 Schottky diodes for potential applications in harsh radiation conditions.

TM-TuP-2 Anisotropic Photoresponsivity and Deviation from Beer-Lambert Law in Beta Gallium Oxide, ***Md Mohsinur Rahman Adnan***, *D. Verma, S. Dhara,* The Ohio State University*; C. Sturm,* Universitat Leipzig, Germany*; S. Rajan, R. Myers,* The Ohio State University

Polarization-dependent photoresponsivity measurements on (001) β-Ga_2O_3 are modeled by calculating the anisotropic absorption process via the dielectric tensor[1]. Quasiparticle band structure calculations show that three different transitions from topmost group of O^{2-} 2p valance bands to the lowest Ga^{3+} 4s conduction band can occur that contribute significantly to the excitonic spectra[2]. A linear polarizer is utilized in the excitation path to generate photocurrent in (001) β-Ga_2O_3 Schottky diode. Three excitonic transitions corresponding to P_x, mixed P_x/P_z and P_y valance band sates are observed as peaks in the measured photoresponsivity spectra at 4.9eV, 5.2eV and 5.5eV[2]. The intensity of the peaks depends on the linear polarization of the excitation.

This strongly anisotropic absorption process in β-Ga_2O_3 cannot be modeled using a generic absorption coefficient; the Beer-Lambert law is not strictly accurate in an anisotropic dielectric. To model anisotropic absorption, we solve the electromagnetic wave equation using the Berreman[3] matrix and the measured dielectric tensor of β-Ga_2O_3[1]. The Poynting vector versus the linear polarization of the excitation with respect to the a- and b- axes and absorption depth is calculated and used to determine the generation rate and the photoresponsivity spectrum of β-Ga_2O_3. The modeled photoresponsivity matches the experimentally measured 3-peak spectrum and its variation with polarization angle. The simulations confirm that the photon flux in β-Ga_2O_3 over the energy range of interest (4-6eV) does not decay exponentially with depth over the photocarrier collection region, in violation with the Beer-Lambert law.

The exciton Franz Keldysh effect is observed in the photoresponsivity spectra, where exciton absorption peaks red shift with reverse bias[4]. The magnitudes of red shift for the three photoresponsivity peaks are inversely related to the corresponding interband transition energies i.e. the smallest energy transition peak shows the highest amount of red shift. We will discuss the polarization anisotropy of the field-dependent red-shift in terms of the exciton wave function anisotropy and its impact on the Stark shift.

[1]C. Sturm et al., APL Mater. 3, 106106 (2015).
[2]J. Furthmüller et al., Phys. Rev. B 93, 115204 (2016).
[3]D. W. Berreman, J. Opt. Soc. Am. 62, 4, pp. 502-510 (1972).
[4]M. M. R. Adnan et al., Phys. Rev. Appl. 16, 034011 (2021).

TM-TuP-4 Self-Trapped Holes and Polaronic Acceptors in Ultrawide Bandgap Oxides, ***John Lyons***, US Naval Research Laboratory

Although Ga_2O_3 is widely believed to be the most promising ultrawide-bandgap semiconductors, its inability to be *p*-type doped hampers its future applications. Recently, other oxide materials have emerged as potential competitors to Ga_2O_3, but their propensity for hole conductivity is less well known. Here the stability of hole polarons in a set of ultrawide-bandgap oxides (Ga_2O_3, Al_2O_3, $ZnGa_2O_4$, $MgGa_2O_4$, $LiGaO_2$ and GeO_2) is examined and compared, both in pristine material and in the presence of acceptor impurities. Holes spontaneously self-trap in all oxides investigated here, with varying stability. Acceptor impurities further stabilize these trapped holes, leading to large acceptor ionization energies. Hole trapping also leads to characteristic distortions and distinct optical transitions, which may explain some experimentally-observed signals. These results indicate that achieving *p*-type conductivity in any of these oxides is unlikely.

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TM-TuP-5 Modeling for a High-Temperature Ultra-Wide Bandgap Gallium Oxide Power Module, ***Benjamin Albano***, Virginia Tech Center for Power Electronics Systems*; B. Wang, C. DiMarino, Y. Zhang,* Virginia Tech Center for Power Electronics

The ultra-wide bandgap (UWBG) of Ga_2O_3 allows it to achieve over 10-times lower intrinsic carrier concentration than Si permitting Ga_2O_3 devices to operate at much higher temperatures. However, its low thermal conductivity and the associated self-heating could cause the device to exceed its safe operating temperature as prescribed by gate dielectric and packaging material limitations. The objective of this study is to develop a physics-based simulation and computation framework for the co-design of Ga_2O_3 devices and packaging.

Table I outlines the benefits and limitations of different models that are conventionally used for device and packaging design. In the design of the package and the micro-/nano-scale device structures, it is critical to observe the interactions between the two [1] [2]. The traditional package-level FEA simulation usually assumes a uniform power density and junction temperature in the devices, while neglecting the temperature variations in the sub-micron device structures; this variation can be up to tens of kelvin under high-power device operations. Conversely, the typical physics-based TCAD simulation accurately models the electrothermal behaviors within the device but the high computational power required (due to the large difference in length scales between the electrically active regions and the thermal diffusion regions) limits their use when package components need to be considered. These models instead simplify the packaging into nominal boundary thermal resistances, neglecting larger packaging elements in the heat flow path that are critical to overall thermal management and reliability [3].

The simple bottom-side cooled diode shown in Fig. 1. was modeled in ANSYS Workbench, Silvaco 2D TCAD, and Silvaco 3D TCAD. As can be seen in Fig. 2., there were stark differences in the heat distribution between the models. These hot spots are severe reliability liabilities and would need to be accounted for in the package design.

In order to build a platform that accounts for the additional electro-thermal effects while still being practical and efficient, a series of models were built to integrate the physics-based material/device-level simulation with a package-level FEA simulation. These models were then evaluated against more traditional methods of device-package simulation, seen in Table II, to understand the potential benefits of such a method. In end effect, this method would guide both device and package design with the hope of identifying and optimizing the thermal and electric field management needs.

[1] IEEE EDL, vol. 90, no. 6, p. 1065-1076, 2002.

[2] IEEE WiPDA, 2018 p. 287-294.

[3] APL, vol. 115, no. 173508, 2019.

TM-TuP-6 Atomic Surface Structure of Sn doped β-Ga_2O_3(010) Studied by Low-energy Electron Diffraction, ***Alexandre Pancotti,*** Universidade Federal de Jataí, Brazil*; J. T. Sadowski,* Center for Functional Nanomaterials, Brookhaven National Laboratory*; A. Sandre Kilian,* Universidade Federal de Jataí, Brazil*; D. Duarte dos Reis,* Universidade Federal do Mato Grosso do Sul, Brazil*; C. Lubin,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay , France*; A. Boucly,* SPEC, CEA, CNRS, Université Paris-Saclay, France*; P. Soukiassian,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, France*; J. Boeckl, D. Dorsey ,* Air Force Research Laboratory*; M. Shin, T. ASEL,* Air Force Research Lab*; J. Brown, N. Barrett ,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay , France*; T. Back,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay

The surface crystallographic and electronic structure of bulk single crystals of transparent, wide gap semiconductor gallium oxide β-Ga_2O_3(010) has been studied using Spot Profile Analysis Low-Energy Electron Diffraction (SPA-LEED) and X-ray Photoelectron Spectroscopy (XPS). The XPS measurements show typical spectra for Ga_2O_3(010). The surface structure of Sn doped single crystal β-Ga_2O_3 Using quantitative LEED I-V. The surface shows a (1 x 1) LEED pattern without reconstruction. The comparison between experimental I-V curves and theoretical LEED simulations using Green's function formalism indicates the formation of a single surface termination layer. There are significant displacements in the first topmost slab surface, moreover, experiment and theory suggest important atomic rumpling between gallium and oxygen atoms in the topmost surface layers. The surface structure agrees with that predicted by first-principles density functional theory calculations and X-ray photoelectron diffraction.

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