

## SPIE Photonics West 2023, San Francisco, USA

**Daniel Hunter**

Department of Physics, University of Strathclyde, SUPA

SPIE Photonics West 2023 is an annual conference held in San Francisco from the 28<sup>th</sup> January-4<sup>th</sup> of February. The gathering is one of the largest photonics exhibitions in the world, consisting of 96 sub-conferences running simultaneously with an industrial photonics tradeshow. Each sub-conference was separated into a sub bracket with the OPTO bracket consisting of the conference I was selected to present at: Oxide-based Materials and Devices XIV.

I was able to present my work investigating the incorporation of Sn into  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and the impact of the Sn alloying on the optical properties of the material. Using wavelength-dispersive X-ray spectroscopy (WDX) and simultaneous cathodoluminescence (CL) measurements I was able determine the substrate influence on how Sn incorporates into a tin-gallium oxide (TGO) thin film and how the Sn alloying greatly supresses the strong UV emission seen in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> while enhancing blue and green luminescence due to an increased density of gallium vacancies and their subsequent complexes with Sn.

### Plenary talks

Three plenary talks were given as part of the OPTO conference bracket. Firstly, Prof. Rajeev Ram from MIT discussing optical transmission within electronics, specifically the benefits of optical integration in on-chip circuits; current research focusing on photonic components to be used within quantum computing and the realm of photonic electronics integrating with in-vivo detectors e.g neural implants.

The second talk was given by Dr. Emily L. Warren from the National Renewable Energy Lab of the USA. Dr Warren discussed the current limitations with solar cells and the limitations of current multi junction solar cells. She firstly addressed the specific issues with these solar cells e,g current matching requirements, cost; she then detailed her current approach to negating these issues using a three terminal (3T) multi junction cell. This concept consists of two solar cells connected in series however they share a central middle contact or feature an additional back contact. Connecting multijunction solar cells in this way removes the need to current match the two terminals while eliminating some resistive losses of independently wired multi-junctions. Preliminary results showed these 3T cells competing with the efficiency of conventional multijunction solar cells (~30%) yet further experimental evidence is required to see if this 3T design is optimal going forward

Prof. Nicolas Grandjean from Ecole Polytechnique Fédérale de Lausanne in Switzerland presented the final plenary talk titled "Are III-nitride semiconductors also suitable for red emission?" which was the most relevant to the research topics during my PhD. The talk began with a brief history of III-nitride semiconductor uses with LED structures, particularly the high operating efficiency of blue InGaN LEDs. He discussed the capability to use InGaN LEDs for

RGB displays due to the bandgap tunability of InGaN alloys to cover the whole visible spectrum. The major issue with the integration of InGaN within red LEDs addressed during the talk was the tendency for the high InN, InGaN LED structures to produce broadened luminescence resulting in emission blueshifting with increasing current. Currently it is difficult to grow InGaN films with a high enough InN content to compensate this increase or upon semi/nonpolar substrates to negate the quantum confined Stark effect causing the blueshift. Therefore, despite the closing of the 'green gap' with increased green III-nitride LED efficiency the struggle for InGaN red LED emission and growth of high quality, high InN InGaN films must first be addressed before RGB LED micro-displays utilising III-nitrides can be considered feasible

## Selected presentations

### **First-principles simulations of transition metal dopants and impurities in in Ga<sub>2</sub>O<sub>3</sub> and related alloys - Joel B. Varley (Lawrence Livermore National Lab, USA)**

Varley uses hybrid functional (HF) theoretical calculations to determine the behaviour of more exotic impurities/dopants (e.g Hf, Zr, Ta) with Ga<sub>2</sub>O<sub>3</sub> and its alloys with Al<sub>2</sub>O<sub>3</sub>. Through these calculations he was able to determine whether these dopants would prefer to incorporate within the octahedral or tetrahedral Ga site within the lattice, formation energy and the position of these dopants within the material bandgap. For Ga<sub>2</sub>O<sub>3</sub> these dopants were found to act as shallow donors but as the material was alloyed they begin to lie deeper within the bandgap. Results showed that the already commonly used Si is the best donor to achieve *n*-type conductivity within Ga<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub> however Hf was found to be a more suitable dopant for (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> alloys, remaining active for greater Al contents compared to the more commonly used Sn. This talk was particularly interesting for me as Varley had performed HF calculations involved within my presentation, investigating the optical behaviour and incorporation of Sn related defects in Ga<sub>2</sub>O<sub>3</sub> so it was interesting to see how these results would compare with that of the exotic transition metals.

### **Diversity of split Ga vacancies in β-Ga<sub>2</sub>O<sub>3</sub> - Filip Tuomisto (University of Helsinki, Finland)**

The existence of 'split' gallium vacancies is another topic related to my presentation with free electron recombination with these vacancies and Sn complexes attributed to the intense blue emission exhibited in the TGO alloys. These 'split' vacancies are when a gallium atom neighbouring a V<sub>Ga</sub> relaxes into an intermediate site within the β-Ga<sub>2</sub>O<sub>3</sub> lattice, forming two 'split' vacancies at the original vacancy site and gallium site. Using positron annihilation spectroscopy Tuomisto determined that not only are these split gallium vacancies ever present within Ga<sub>2</sub>O<sub>3</sub> crystals but that they are present in very high densities (order of 10<sup>18</sup> cm<sup>-3</sup>). Further to this two intentionally doped Ga<sub>2</sub>O<sub>3</sub> crystals were investigated containing Sn & Fe dopants. It was found that the density of the split gallium vacancies was reduced within the Fe doped material yet Sn doped Ga<sub>2</sub>O<sub>3</sub> had an increased density. If this trend stayed true for the high Sn content TGO alloy then it would reinforce our claim that these split vacancies may be responsible for the intense blue emission seen in our samples.

**Role of hydrogen in gallium oxide** - *Chris G. Van de Walle (University of California, Santa Barbara, USA)*

It was first explained that  $\text{Ga}_2\text{O}_3$  will always contain hydrogen regardless of the growth method used: whether coming from the precursor material in MOCVD growth or contamination within chamber walls in MBE. Similarly to Varley's presentation HF calculations were performed to determine hydrogen formation within  $\text{Ga}_2\text{O}_3$  distinguishing between the occurrence inside the crystal and as a surface impurity. Focus was particularly directed on the ability for hydrogen to form complexes with impurities in the material bulk. The formation of these hydrogenated complexes was shown to be extremely probable with complexes exhibiting different optical properties depending on the degree of passivation. This was again relevant to my work as similar calculations were performed to determine the formation of hydrogenated Sn complexes possibly responsible for red luminescence from TGO films.

**Crucible free growth of oxide crystals** - *Kei Kamada (Tohoku University and C&A Corporation, Japan)*

The ability to grown bulk single crystal  $\text{Ga}_2\text{O}_3$  material removes the need for non-native substrates for epitaxial growth. Kamada detailed the issues with the current growth methods: the requirements for iridium crucibles results in the  $\text{Ga}_2\text{O}_3$  product being expensive and containing Ir impurities as well as the crystals containing a high density of oxygen vacancies with the current methods. Kamada details his new growth method "oxide crystal growth from cold crucible (OCCC)". This new method replaces the need for the iridium crucible by containing the  $\text{Ga}_2\text{O}_3$  precursor in a water cooled basket and uses a number of high frequency magnetic coils as a heating source. With this set up the inner core of the raw material is sufficiently heated simultaneously with adequate cooling of the outer material allowing stable growth. From this large  $\text{Ga}_2\text{O}_3$  cylinders up to 5cm diameter can be grown from a seed crystal. Closing remarks summarised how the OCCC method may be used not only to produce low-cost, Ir free  $\text{Ga}_2\text{O}_3$  material but other oxides too e.g. YAG ( $\text{Y}_3\text{Al}_5\text{O}_{12}$ ).

**Phase stability of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  polymorphs: a first-principles study** - *Sai Mu (University of South Carolina, USA)*

For low levels of Al alloying,  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys take on the monoclinic ( $\beta$ -) structure however depending on the alloy composition the stability of other polymorphs [corundum ( $\alpha$ ), orthorhombic ( $\kappa$ ), and defective spinel ( $\gamma$ )] increases. Mu uses DFT calculations to investigate the stability and formation probability of the four mentioned  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  polymorphs as a function of alloy composition and temperature, 0-1400K. Enthalpy of formation calculations determine that at 0K for the  $\beta$  &  $\kappa$  phases of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  an Al content of 50% results in the greatest stability of the polymorph and 62.5% for  $\gamma$ - material.  $\alpha$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  stability continues to increase with the greatest being for pure  $\text{Al}_2\text{O}_3$ . For temperatures  $\geq 1400\text{K}$  DFT calculations indicate that the  $\beta$ -polymorph is the most stable for Al contents  $< 50\%$  and  $\kappa$ -phase the second most stable. Mu concluded by saying that theoretical results agree with experimental work on bulk single crystal materials but not with epitaxial  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3$  thin films where multiple polymorphs are observed, particularly  $\gamma$ -phase, suggesting additional kinetic factors outside of strain may be responsible.

## Conclusion

I'd like to thank the UKNC for their financial support allowing me to attend this conference. This provided me with the opportunity to not only present the results of my studies but to listen to what other students and researchers from across the world are doing to further the field. I was also able to network with many photonic based companies attending as part of the accompanying tradeshow discussing future career opportunities and observe demonstrations of the latest products in photonic technology.