European Materials Research Society(E-MRS) Fall meeting 2023 Conference Report Mugove Maruzane Semiconductor spectroscopy group, Strathclyde University, Glasgow, United Kingdom <u>mugove.maruzane@strath.ac.uk</u>

Introduction

The European Material Research Society held a conference that was split into five main categories which are information and communication technologies, energy and environment, manufacturing, health and fundamentals. In these five categories, 25 symposiums were held and the main symposium that I attended was the ultrawide bandgap semiconductors for energy and electronics symposium that was under energy and environment in symposium E.

The conference started on Monday the 18th of September and for Monday and Tuesday the conference had two morning sessions that were divided by a coffee break and 2 afternoon sessions that were also divided by a coffee break. On Wednesday plenary talks were held in the morning followed by two afternoon sessions. On Thursday which was the last of the conference, there were 2 morning sessions and a single afternoon session. Every session at the conference was started by a 30-minute invited talk followed by 15-minute talks. On Wednesday there were only 3 45-minute talks that where held in the main hall.

My presentation was on the cathodoluminescence of epitaxy lateral overgrown gallium oxide which I had presented at the UWO conference in Bristol and I am planning to present at the next UKNC conference to be held at Strathclyde University. I was given a 15-minute slot on the final day of the conference. I greatly enjoyed the conference and I managed to meet some people that are working on gallium oxide. Below are some presentation that I took some interest into and that I felt may be helpful in my research.

Title: Effect of hydrogen in Si-doped beta-gallium oxide grown by liquid injection MOCVD

Speaker: Fridrich Egyenes

Affiliation: Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava, Slovakia - Bratislava (SLOVAKIA) - Bratislava (Slovakia)

Type: Talk

In the talk the speaker introduced gallium oxide to the audience. They mentioned that gallium oxide has a bandgap of 4.8 eV which makes it a potential candidate for high power applications. Then went on to discuss how hydrogen atoms are capable of forming donors in gallium oxide and how they can theoretically affect the properties of gallium oxide. The samples used in the talk where silicon doped samples that had hydrogen incorporation and they where grown on c-plane sapphire. Thickness of

the samples was measured by ellipsometry and were reported to have a thickness in the range of 140-200nm. The experiment also showed that higher temperature growth leads to better quality samples up to a temperature of 700 degrees and from then on, the samples seemingly start to degrade. The also mentioned that they noticed some degradation happening from the edges of the sample. They also tested the conductivity of various samples that where annealed at different temperatures and also with varying oxygen flow. They noticed that conductivity improved with increasing annealing temperature and it also improved with increasing oxygen flow.

Title: Growth and Ambient-driven Crystalline Phase transition in Ga2O3 thin films

Speaker: Armit Khare

Affiliation: School of Physics, Trinity College Dublin - Dublin (Ireland), 2AMBER Centre & Centre for Research on Adaptive Nanostructures and Nanodevices, Trinity College Dublin - Dublin (Ireland)

Type: Talk

The talk opened up on a brief of the general properties of gallium oxide and the motivations for growing gallium oxide via pulsed laser epitaxy. The gallium oxide samples that that were the subject of the research were grown using pulsed laser epitaxy at a temperature of 800 degrees Celsius on MgO substrates in oxygen and they yielded gamma and beta gallium oxide think films. XRD was performed on the samples however the presenter highlighted that XRD is not sufficient in differentiating gamma and beta gallium oxide so Raman scattering was then performed on the samples and the active modes known to be present in beta gallium oxide were not present in gamma gallium oxide despite the high temperature growth process.

Title: New material for power devices: GeO2

Speaker: Kaneko

Affiliation: Ritsumeikan University - Kusatsu (Japan)

Type: Talk

In the presentation they introduced the importance of ultra-wide bandgap semiconductors and they advantages in the processing of high-power devices. They also discuss how germanium oxide is an alternative to gallium oxide and can be advantageous since it has the ability to form p type conductivity which is difficult to form in gallium oxide, however they also highlight the difficulties faced with growing highly crystalline germanium oxide. The presenter shows how they managed to achieve a stable growth method of growing germanium oxide at a rate of 1micormeter per hour using mist chemical vapour deposition. The growth was achieved by inject a large amount but the thin films still contained areas with poor crystal quality when observed in TEM. The rutile structure of germanium oxide was discussed as having a similar formation energy as the formation energy of amorphous phase germanium oxide. The presenter suggested performing more studies on germanium oxide and also investigating the effects of alloying on germanium oxide.

Title: **Complex gallium oxide polymorphs explored by accurate and general-purpose machine** *learning*

Speaker: Junlei Zhao

Affiliation: Southern University of Science and Technology - Shenzhen (China)

Type: Talk

Due to the complex nature of some gallium oxide polymorphs and their low symmetry some information that relates to the properties of some gallium oxide polymorphs maybe missed henceforth the presenter developed a kernel-based machine learning approximation for gallium oxide. Molecular dynamics is the preferred computational method for gallium oxide and it is mainly reliant on how the atomic force between molecules is calculated. The machine learning gaussian approximation (ML-GAP) showed a straight line with DFT data. Two versions of interatomic potentials where realised namely soapGAP and tabGAP. soapGAP was 400 times faster and tabGAP was 20000 times faster than DFT calculations. The machine learning had a very good predication of the data with a slight deviation from the DFT data. The presenter also touched on the atomic mechanism of converting beta phase into gamma phase in a solid-state phase change that is induced by an ion beam. Gamma phase has a tetrahedral structure but gallium oxide prefers an octahedral structure. This therefore results in a polymorphic layer that can enable special properties in gallium oxide.

Title: Modelling properties of gallium oxide-based quantum structures to achieve hole conductivity

Speaker: Tamar Tchelidze

Affiliation: Ivane Javakhishvili Tbilisi State University - Tbilisi (Georgia)

Gallium oxide is presented has having low hole mobility which reduces functionality of gallium oxidebased devices. This can be improved by implementing quantum structures into the gallium oxide thin film which where model in the case of this presentation. The main quantum structure that was modelled for the presentation is the triangular confinement potential. The triangular potential well is a widely adopted geometry due to its similarity to the potential profile observed in quantum heterojunctions. They investigated near surface holes in the presence of an electric field and the surface conductivity was related to the surface defects. The surface accumulation was classified as accumulation, depletion, flat bands and inversion. The potential well was unable to accommodate holes and the coulomb potential was reduced to 1 dimension, the singularity removed effective radius defined based on a 2D coulomb solution. There was an observable shift in the valence band due to the presence of the electric field, the energy wells where quantized, bandgap was reduced and acceptor ionization energy was also reduced which could improve p-type conductivity in gallium oxide.

Title: Exploration of Zirconium doping in pulsed laser deposit in alpha-gallium oxide

Speaker: Sofie Vogt

Affiliation: Felix Bloch Institute, University Leipzig - Leipzig (Germany)

The presenter touched on the benefits of alloying alpha gallium oxide with other semiconductor oxides like indium, tin and aluminium oxide. Their samples were grown via pulsed laser deposition with and unintentionally doped alpha gallium oxide seed layer grown at a higher temperature and the zirconium doped alpha gallium oxide grown at a temperature lower than 600 degrees. The resultant films had a small window of conductivity and the lower the dopant the larger the window of conductivity became. The best films where discovered to occur at a growth temperature of 450

degrees, lower growth temperature resulted in a lower crystal structures and higher growth temperatures resulted in different growth mechanism. The films had an electron mobility of 38cm/Vs. The zirconium incorporation was higher towards the surface of the film which differs from what has been observed in with silicon and tin doping. The increase of the amount of Zirconium in the film also resulted in an increase in the etch time for the thin film.