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MOCVD Al(Ga)N Insulator for Alternative Silicon-On-Insulator Structure

Glenn Ross
Department of Electrical Engineering
and Automation
Aalto University
Espoo, Finland
glenn.ross@aalto.fi

Ville Luntinen
Department of Electrical Engineering
and Automation
Aalto University
Espoo, Finland
ville.luntinen@gmail.com

Mikael Broas
Department of Electrical Engineering
and Automation
Aalto University
Espoo, Finland
0000-0002-9339-5069

Sami Suihkonen
Department of Electronics and
Nanotechnology
Aalto University
Espoo, Finland
sami.suihkonen@aalto.fi

Turkka Tuomi
Department of Electronics and
Nanotechnology
Aalto University
Espoo, Finland
turkka.o.tuomi@aalto.fi

Aapo Lankinen
Department of Electronics and
Nanotechnology
Aalto University
Espoo, Finland
aapo.lankinen@okmetic.com

Andreas Danilewsky
Kristallographie, Institut für Geo- und
Umweltnaturwissenschaften
Albert-Ludwigs-Universität
Freiburg, Germany
a.danilewsky@krist.uni-freiburg.de

Markku Tili
Okmetic Oy
Vantaa, Finland
0000-0001-6953-3153

Mervi Paulasto-Kröckel
Department of Electrical Engineering
and Automation
Aalto University
Espoo, Finland
mervi.paulasto@aalto.fi

Abstract— Due to the functional limitations of SiO₂ for SOI applications, alternative dielectric materials have been investigated. Alternative SOI materials in this work include, AlN and AlGa_{0.5}N. The dielectrics were deposited using MOCVD, and with the aid of PECVD deposited SiO₂, and the SiO₂ was directly bonded to a handle Si wafer. Tensile tests were performed on the samples to examine the fracture behavior and maximum tensile stresses, with results being comparable to a traditional SOI. Characterization was undertaken using TEM to understand the microstructural and interfacial properties of alternative SOI. High crystal quality Al(Ga)N was achieved on a Si(111) substrate that generally contained well defined chemical interfaces. Finally, synchrotron X-ray diffraction topography was used to understand the topographical strain profile of the device and handle wafers. Topography results showed different strain network properties between the device and handle wafer. This work has demonstrated preliminary feasibility of using alternative dielectrics for SOI applications.

Keywords—silicon-on-insulator, dielectric, metalorganic chemical vapor deposition, direct bonding, aluminum nitride, aluminum gallium nitride, tensile tests, transmission electron microscopy, synchrotron x-ray diffraction topography.

I. INTRODUCTION

Silicon-on-insulator (SOI) is the backbone of multiple silicon-based technologies that include traditional integrated circuit (IC) technologies, silicon based microelectromechanical systems (MEMS), radio frequency (RF) applications and silicon photonics. The principle of SOI is to use a thin dielectric layer, traditionally consisting of SiO₂, to isolate the device layer from the substrate bulk. This results in several functional advantages for IC technologies; it also spawned several SOI variations for targeted applications, such as cavity-SOI for the simplification of MEMS fabrication [1].

Decarbonization by the electrification of things, miniaturization and increased switching speeds of devices is challenging thermal management of ICs. Dense architectures with embedded 3D structures are exacerbating hot-spot and

self-heating issues. Thermal management is playing an ever-important role in material selection and design. The use of SiO₂ as an insulating layer does not allow for the efficient redistribution of heat due to its low thermal conductivity. There are several potential alternatives to SiO₂, including aluminum nitride (AlN), aluminum gallium nitride (AlGa_{0.5}N), and alumina (Al₂O₃), that have superior thermal conductivity. To put the magnitude of difference in perspective, the thermal conductivity of SiO₂, AlN, and Al₂O₃ is 1.4, 319, and 18W/m.K respectively, which in the case of AlN is over a 200 fold increase over SiO₂. This work proposes alternative dielectric materials, such as AlN and AlGa_{0.5}N that exhibit significantly better thermal conductivity than SiO₂ [2][3][4].

As promising as these materials are for an alternative SOI application, an understanding of the thermomechanical and thermodynamic behavior is crucial. For example, how the deposition process affects crystal quality and subsequently the functional properties of the dielectric. This work is an early demonstration of using alternative materials for a SOI application. Metalorganic Chemical Vapor Deposited (MOCVD) AlN and AlGa_{0.5}N are used as an alternative dielectric to study the mechanical and microstructural performance of alternative SOI. Tensile measurements determine whether there are any negative thermomechanical effects of having a polycrystalline dielectric compared with amorphous SiO₂. The microstructural and strain properties are examined to understand the effects of MOCVD grown Al(Ga)N, and possible challenges related to residual stresses and strain networks at growth and bonding interfaces.

II. MATERIALS AND METHODS

A. Alternative SOI Fabrication

MOCVD AlN and AlGa_{0.5}N layers were grown on DSP Si(100) and Si(111) device substrates at growth temperatures over 1000°C. Currently there is no optimized process in the lab for polishing and bonding Al(Ga)N directly to silicon, therefore Plasma Enhanced Chemical Vapor Deposited (PECVD) SiO₂ was introduced to run the standard SiO₂-Si

bonding process. A 500nm layer of PECVD SiO₂ was deposited and annealed to remove excess hydrogen from the film to avoid void formation during bonding [1]. A Chemical Mechanical Polishing (CMP) and wafer cleaning process were undertaken to provide a suitable surface roughness for the direct bonding of the SiO₂ surface. Direct bonding between the SiO₂ polished surface and an SSP Si(100) handle wafer was carried out, followed by a post bonding anneal. Finally, the device wafer was thinned towards the Al(Ga)N growth interface. Fig. 1 illustrates the process flow and a list of the samples, substrate type, and thicknesses can be found in TABLE I.

Fig. 1. Shows the general process flow for the alternative SOI platform. (i) is the deposition of Al(Ga)N on Si (ii) is the deposition of PECVD SiO₂, polishing and cleaning (iii) is the bonding process including post-bonding annealing and (iv) is final thinning of the device substrate revealing the final structure for characterization.

TABLE I. OVERVIEW OF THE SAMPLE NUMBER, SAMPLE STRUCTURE, SUBSTRATES AND THICKNESSES OF THE LAYERS

Sample Structure	Handle Si	Device Si	SiO ₂ [nm]	Al(Ga)N [nm]
1 Si/SiO ₂ /AlN/Si	(100)	(100)	130.5 ± 2.9	205.0 ± 2.9
2 Si/SiO ₂ /AlN/Si	(100)	(111)	253.8 ± 0.3	206.8 ± 0.2
3 Si/SiO ₂ /AlN/Si	(100)	(100)	206.4 ± 3.2	206.0 ± 3-2
4 Si/SiO ₂ /AlN/Si	(100)	(111)	201.5 ± 0.3	126.6 ± 0.3
5 Si/SiO ₂ /AlGaN/AlN/Si	(100)	(111)	208.0 ± 0.1	202.2 ± 0.8

B. Tensile Test

Tensile tests were carried out using an MTS 858 Table System using a Flex Test 40 digital control and an MTS SilentFlow HPU system (Fig. 2 (i)). The tensile test was based on a stud pull method. Sections of the bonded wafers were diced into $4.8 \times 4.8 \text{ mm}^2$ squares using a wafer dicer (Disco DAD3220). The diced sample pieces were mounted and glued between brass pull studs (Fig. 2 (ii)) using high-strength epoxy glue (Loctite® Power Epoxy Universal). Once the glue had hardened, the studs were mounted into the stud holders (Fig. 2 (iii)) and loaded into the tensile tester using hydraulic grippers.

Fig. 2. Is an overview the tensile test setup. Subfigure (i) is the MTS 858 table system, (ii) are the bonded sstamples glued to the studs and (iii) are the stud holders.

The tensile pull rate applied to the samples was 0.01mm/s and a sample population of 30 samples per wafer was chosen for statistical significance. All samples were measured until fracturing occurred. Optical fracture surface analysis was carried out to determine the fracture mode.

C. Microstructural Characterisation

Samples for the microstructural characterization were prepared by first molding and cross-sectioning the bonded samples using a standard metallographic cross-sectioning procedure. The samples were pre-molded and cross-sectioned because the thinned device substrate was too thick to directly prepare a TEM lamella. TEM lamellas were prepared from the molded cross-sections using a dual-beam (FIB-SEM) JEOL JIB-4700F using an *in-situ* lift-out process. Transmission electron microscopy (TEM), scanning transmission electron microscopy (STEM), select area electron diffraction (SAED), and energy-dispersive X-ray spectroscopy (EDS) were conducted using the JEOL JEM-2800 operating at 200kV.

D. Synchrotron X-ray diffraction topography

Synchrotron radiation X-ray diffraction topography (SR-XRT) is a highly strain sensitive method for imaging (topographs) selected areas of single crystalline material. The measurements were recorded at the TOPO-TOMO beamline at ANKA (Angstromquelle) in Karlsruhe [5]. The energy-dispersive diffraction diffracts several topographs from the irradiated volume onto an X-ray sensitive film. In energy dispersive mode, photons of energy E diffracts by lattice planes of interplanar spacing d when the Bragg condition is fulfilled (seen in equation 1), where h is Plank's constant, c is the speed of light and θ is the half angle.

$$hc/E = 2d \sin(\theta) \quad (1)$$

There are two main modes of operation, (i) back-reflection mode and (ii) transmission mode, which are illustrated in Fig. 3. In back-reflection mode, the diffracted pattern is collected at $<90^\circ$ from the incident beam and the transmission mode collects the sample transmitted beam. The Laue diffraction pattern on the film is Miller indexed, enlarged using an optical microscope, and digitized. A detailed explanation of the method with similar samples can be found in [6].

Fig. 3. Illustrates the (i) transmission mode and (ii) back-reflection mode of the SR-XRT setup. The Laue diffraction pattern from the single-crystal samples are projected onto the X-ray sensitive film. Adapted from [7].

III. RESULTS AND DISCUSSION

A. Tensile Test

The results of the tensile measurements are summarized in TABLE II. On average, a tensile strength of 15.9MPa from all the samples was measured. This corresponds well with reported values in the literature of Si-Si or Si-SiO₂ directly bonded samples, which appear to be within the range of 10-15MPa [8][9][10]. This indicates that there are no negative effects of using Al(Ga)N in a SOI structure; such as a weak adhesion at the dielectric growth interface or intergranular fracturing of the polycrystalline Al(Ga)N.

TABLE II. TENSILE TEST RESULTS

Sample Structure	Avg. F [N]	Std. Dev. [N]	σ [MPa]	Relative Std. dev. [%]
1 Si/SiO ₂ /AlN/Si	262.5	56.5	11.4	21.5
2 Si/SiO ₂ /AlN/Si	382.6	62.0	16.6	16.2
3 Si/SiO ₂ /AlN/Si	260.7	53.8	11.3	20.6
4 Si/SiO ₂ /AlN/Si	365.6	78.9	15.9	21.6
5 Si/SiO ₂ /AlGaIn/Si	385.5	82.2	16.7	21.3

There are several challenges associated with the stud pull test. These include, inconsistent gluing resulting in glue failures, glue overflow resulting in glue bonding of brass studs and shear loading of an incorrectly mounted samples leading to uneven tensile loading. Fracture surface analysis characterized the resulting fracture behavior, shown in Fig. 4. Four primary failure modes had been identified, (I) clean fracture, from the bonding interface (Si-SiO₂), (II) partial fracture, a combination of glue-line fracture and bond failure, (III) glue-line fracture, failing of the glue and (IV) through-sample partial fracture. Most of the samples exhibited failure modes I, II or IV (82%). However, a significant fraction were caused by the glue-line fracture (18%), failure mode III. As these exhibited unrealistic tensile strength results, they have been excluded from the results found in TABLE II.

Fig. 4. The figure shows the different types of fracture modes that occurred during tensile measurements, (i) is a clean fracture, (ii) is a partial fracture, (iii) is a glue-line fracture and (iv) is a through-sample partial fracture.

B. Microstructural Characterization

The microstructural characterization study determines the (i) crystal quality of the Al(Ga)N, (ii) chemical state, (iii) Al(Ga)N growth interfaces, and (iv) bonding interface. The results for the crystal quality can be seen in Fig. 5. In general, Al(Ga)N grown on Si(111) compared with Si(100) is of significantly higher crystal quality. For example, for AlN grown on Si(100) in Fig. 5 (i) a clear polycrystalline microstructure (grain size ~20nm) is observed and Fig. 5 (iii) a wider distribution of the AlN(0002) around the substrate normal indicating a lower crystal quality. In contrast, AlN grown on Si(111) in Fig. 5 (ii) exhibits much larger columnar grain structure (grain size ~100nm) and Fig. 5 (iv) a tightly bound distribution around the device substrate normal. Although there is significant lattice mismatch between Si(111) and AlN(0002), this can be relaxed, for the Si(111) surface, by an array of misfit dislocations propagating from the growth interface [11].

Fig. 5. STEM results from (i) AlN grown on Si(100) and (ii) AlN grown on Si(111). Figures (iii) and (iv) are their respective SADP. The selected area for the SADP was generated from the device Si and AlN regions only.

A summary of the sample crystal quality and Al(Ga)N/SiO₂ interfacial roughness can be seen in TABLE III. The roughness of the Al(Ga)N layer is of interest. In a subsequent run of experiments, the aim would be to bond Al(Ga)N directly to Si handle. Ideally, from a processing and performance point-of-view, it would be advantageous to bond the dielectric layer directly with Si with a minimum of pre-processing steps (i.e. grinding, CMP, cleaning, etc.). A critical direct bonding parameter is the surface roughness, which ideally needs to be below 0.5nm [1] to achieve a good bond. Although slightly above this value (for Al(Ga)N grown on Si(111) wafers), only a minimal surface preparation could be required to achieve a successful direct bond.

TABLE III. OVERVIEW OF THE AL(GA)N FILM QUALITY AND AL(GA)N/SiO₂ INTERFACIAL ROUGHNESS (RMS)

Sample Structure	Al(Ga)N (002)	R _{q1}
	[arcsec]	[nm]
1 Si/SiO ₂ /AlN/Si	49256	9.4
2 Si/SiO ₂ /AlN/Si	7034	0.9
3 Si/SiO ₂ /AlN/Si	56826	10.2
4 Si/SiO ₂ /AlN/Si	10250	1.0
5 Si/SiO ₂ /AlGa _{0.15} N/Si	8168	0.5

An example of the EDS chemical analysis of two samples can be seen in Fig. 6. Generally, all interfaces exhibit well-defined chemical interfaces with little to no interdiffusion of species. However, it has been observed at specific Al(Ga)N grain boundaries (indicated in the figure with a white arrow) the diffusion O into AlN, which can be seen along the SiO₂/AlN interface in Fig. 6 (i). With the AlGa_{0.15}N sample there is an AlN layer followed by an AlGa_{0.15}N. The AlGa_{0.15}N epilayer requires a buffer layer to handle the lattice mismatch between Si and AlGa_{0.15}N layers. An EDS point analysis of the Al_xGa_{1-x}N_y showed a composition of $x = 38.7$ and $y = 51.7$.

Fig. 6. STEM-EDS results from (i) sample 2 and (ii) sample 5 with the AlGa_{0.15}N layer. Small white arrow indicates region of diffusion of O into AlN.

A high-resolution study of the growth interface of AlN on the Si(111) surface reveals a thin amorphous layer (~3-5nm thick), seen in Fig. 7 (i). Above the amorphous layer is a thin layer (10-20nm thickness) of miss-orientated grains that are quickly accommodated to form highly c-axis orientated AlN, similar to the behavior observed in [11] and [12]. Fig. 7 (ii) shows the interface between SiO₂ and AlN with no significant defects, apart from the earlier described O diffusion into AlN.

Fig. 7. HRTEM micrographs from (i) the device Si(111) and AlN growth interface and (ii) PECVD SiO₂ growth interface.

The bonding interface of Si/SiO₂ is presented in Fig. 8 and shows that the hydrophilic wafer bonding process had formed a defect void-free interface.

Fig. 8. HRTEM micrographs of the handle Si and SiO₂ bonding interface.

C. Synchrotron X-ray diffraction topography

An image of the Laue diffraction back-reflection mode X-ray sensitive film recorded at ANKA can be seen in Fig. 9. Reflections for both the device and handle substrates are visible in the film. Superimposed on the image are the Miller indices for the device substrate (red) and the handle substrate (blue). The darker regions of the film represent the topographs from a specific reflection. Within the region of one reflection, there are lighter and darker areas. The darker regions within a reflection correspond to an area of higher strain with respect to the lighter areas. More details of the technique are provided in [13].

Fig. 9. (i) Schematic representation of the back-reflection topography measurement using X-ray sensitive film. The continuous wavelength x-ray beam (blue) traverses the hole in the film and is simultaneously diffracted back (green) onto the film by several sets of lattice planes in both the handle and device layers (Adapted from [13]). (ii) is the X-ray sensitive film Laue diffraction under back-reflection mode. Shown in the image are the indexed reflections from the device substrate (red) and handle substrate (blue).

The magnified 100 reflection from the transmission and 312 from the back-reflection mode topographs can be seen in Fig. 10 (i) and (ii), respectively. The handle substrate (Fig. 10 (i)) exhibits much larger cells with borders that are less distinctive indicating a possible smaller strain, much like those observed in regular SOI wafers [6], as bonding and post bonding annealing temperatures are significantly lower. The topograph of the device substrate (Fig. 10 (ii)), on the other hand, shows a cellular network of strongly strained borders. Significant strain at the Al(Ga)N growth interface is expected due to the high deposition temperatures required for MOCVD, the mismatch between the coefficients of thermal expansion (CTE) of Si and Al(Ga)N and the lattice mismatch between Si(111) and AlN(0002).

Fig. 10. Are topographs from sample 5, (i) is the 100 large-area transmission-reflection topograph from the handle substrate and (ii) is the 312 large-area back-reflection topograph from the device substrate.

The next logical step for an understanding of the strain profile in alternative SOI structures is to (i) directly bond Al(Ga)N to Si and understand the change in the strain profile of the device substrate and (ii) examine the samples using a topograph section, which provides a more quantitative indication of the magnitude of strain in the device and handle wafers.

IV. CONCLUSION

In conclusion, this work has presented a study into the mechanical and microstructural properties of an alternative SOI demonstrator. The results have shown that alternative

SOI samples have exhibited average tensile strength of 15.9MPa, comparable to the more traditional buried oxide SOI. This shows that there are, in principle, no undesirable effects of having a polycrystalline dielectric layer.

A microstructural study showed the crystal properties of MOCVD grown Al(Ga)N, which exhibits high crystal quality when grown on a Si(111) substrate. In general, all films exhibited chemical stability, however in some cases there was diffusion of O into the AlN at grain boundaries. Synchrotron X-ray diffraction topography studied the strain profile differences between the handle and device substrates. The handle wafer exhibited a larger less distinctive network of strain cells compared with the device wafer, indicating a more significant strain in the device layer. The strain is generated due to the high processing temperatures of the MOCVD deposited Al(Ga)N, CTE mismatch, and the lattice mismatch.

Finally, the next logical steps in the study to determine the suitability of alternative dielectrics, such as AlN or AlGa_{0.5}N, for SOI applications is the removal of the SiO₂. There are several technical and theoretical challenges that need to be overcome for the reliable implementation of alternative SOI. Some of these currently under consideration are the AlN-Si direct bonding behavior and the thermomechanical performance. Nonetheless, there are clear performance and processing gains possible with an alternative SOI platform justifying continual research and development of the topic.

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