Virtual substrates for wide bandgap $Al_yX_{1-y}N$ growth

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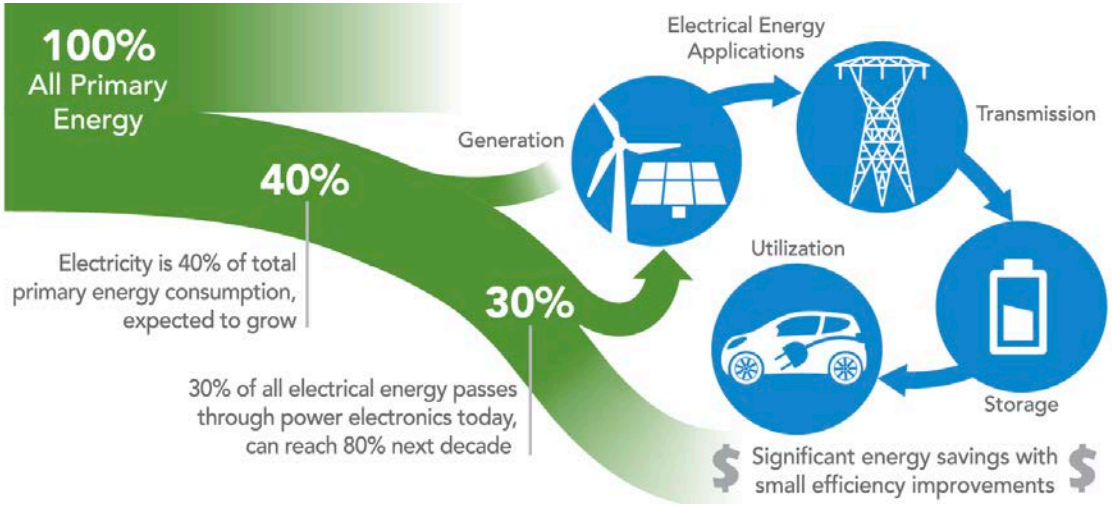
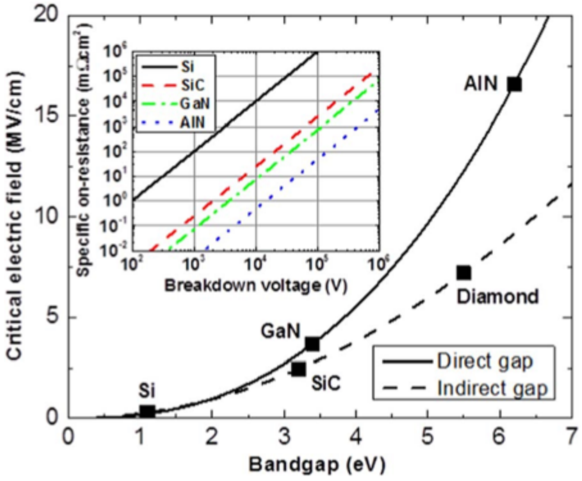
6 Mar 2024

Session M64: Optoelectronic and Photovoltaic Energy Conversion

Increased electrification drives the need for power electronics



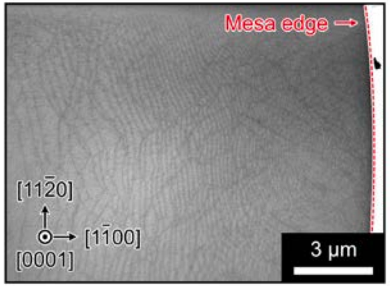
Why AlGaN?



- Larger band gaps (ultra-wide!) enable larger electric fields
  - p- and n-dopable
  - high mobility and stability
  - Mature growth processes

Reese et al., Joule 3, 899–907, April 17, 2019
Kaplar et al., 2017 *ECS J. Solid State Sci. Technol.* **6** Q3061

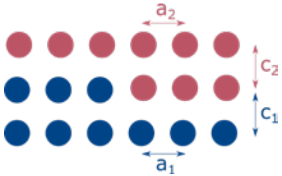
The effect of the substrate

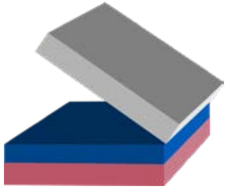


Main deployment barrier: lattice mismatch causing layer cracking and dislocations, impacting optical and electrical properties

< Dislocations in AlGaN on AlN device – Kumabe et al, IEEE Trans. on Electronic Devices 2024

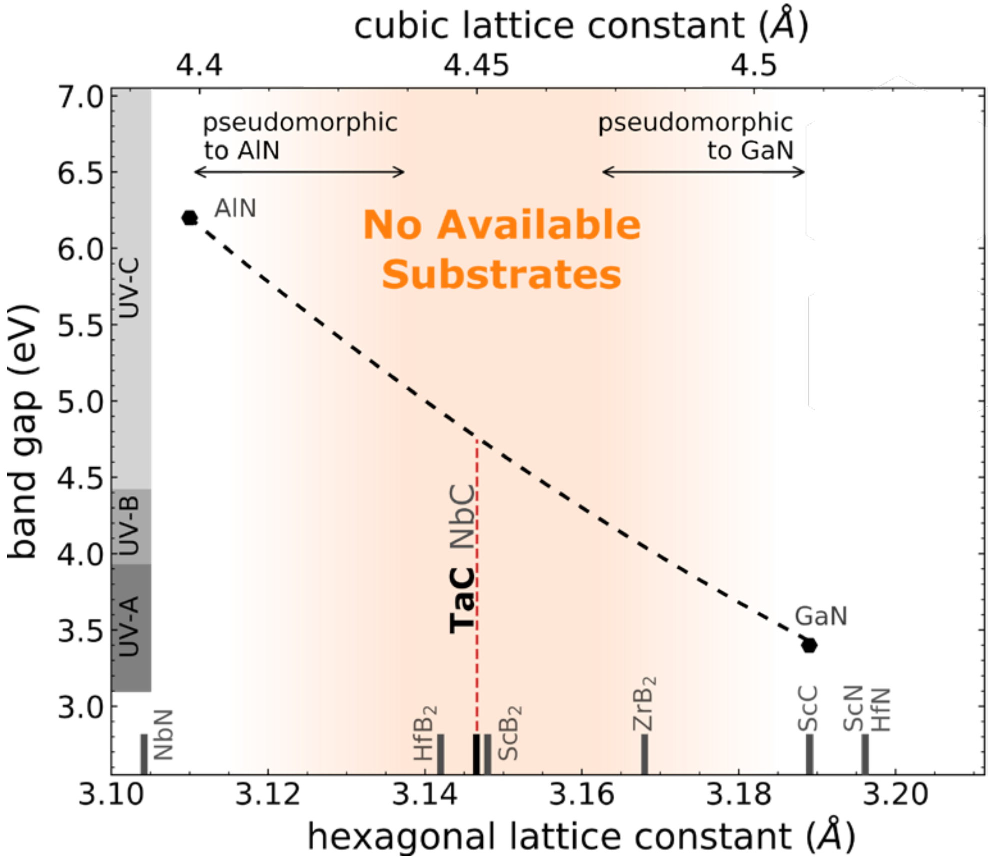
Properties of an ideal substrate





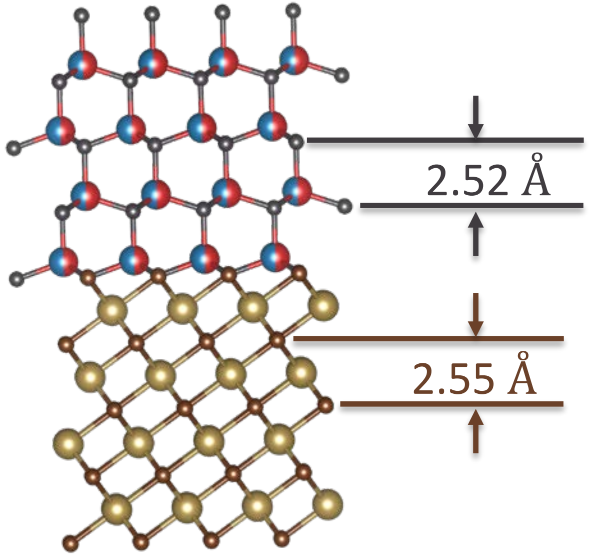
- Lattice matched – both in-plane (atomic registry) and out-of-plane (step height registry)
- Thermal-expansion matched – growth temperature and cooling
- Scalability – low-cost manufacturing techniques
- Device compatibility – electrically conductive with good thermal conductivity for vertical devices
- Bonus – chemically/optically dissimilar for substrate removal

Transition metal carbides are lattice matched to AlGaN



- (111) TaC is lattice matched to $Al_{0.45}Ga_{0.55}N$ (0001)
- Potential tunability via process parameters and alloying!

Transition metal carbides are lattice matched to AlGaN



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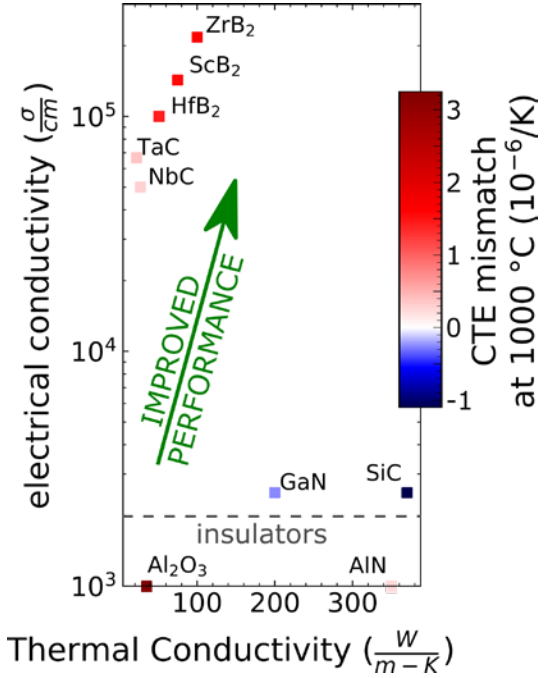
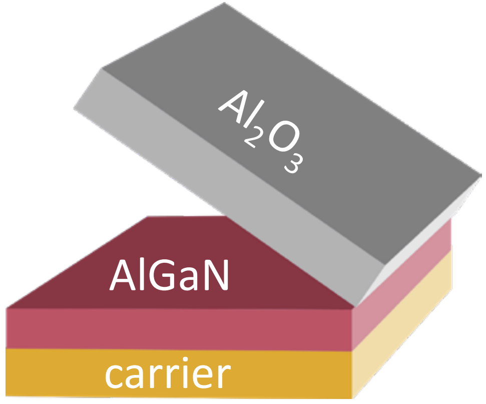
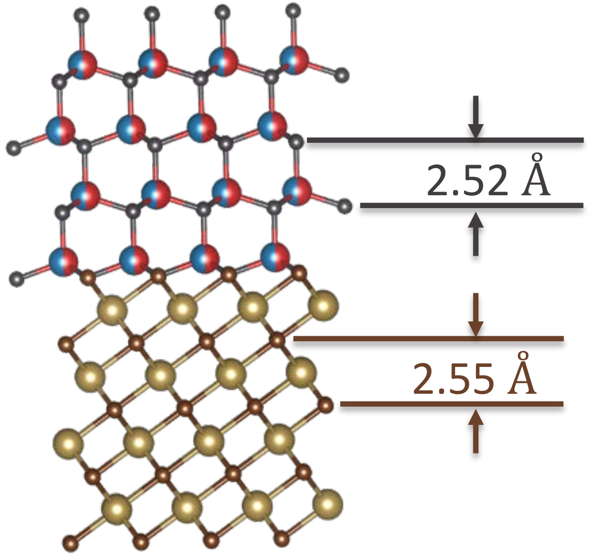


Conductive with compatible CTE



Chemically dissimilar – potential for substrate removal

Transition metal carbides are lattice matched to AlGaN



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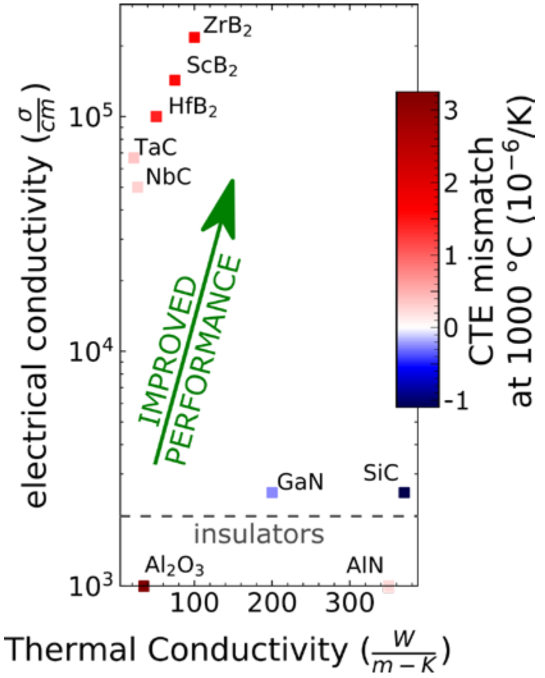

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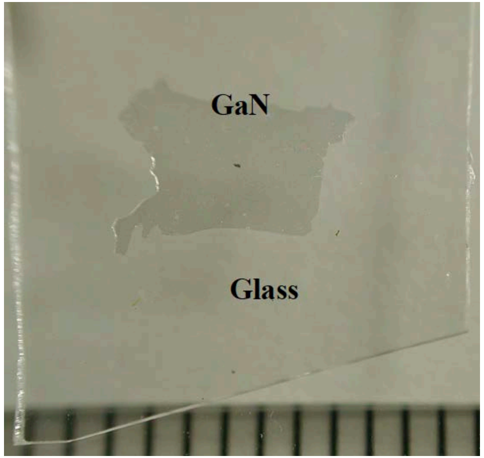
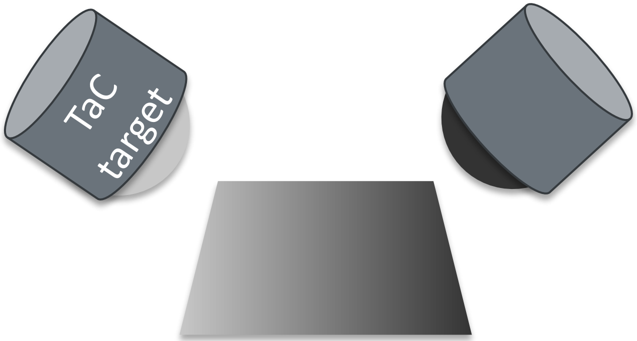


Freestanding GaN removed from ZrB_2

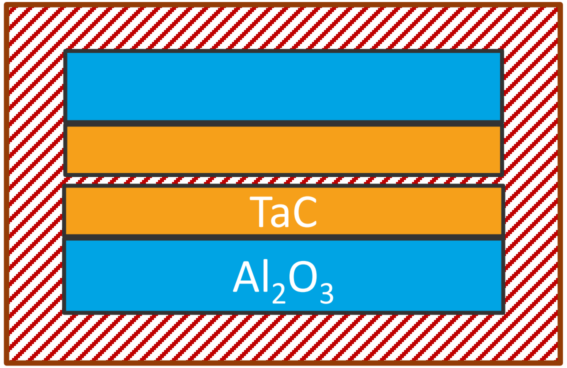
Hiroshi Amano et. al., Proc. SPIE 2003

Approach



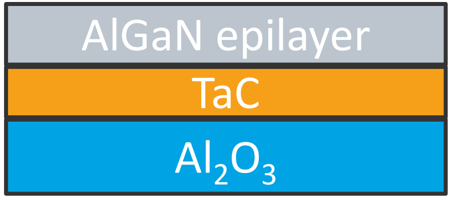
Step 1: sputter deposition

Grow epitaxial TaC



Step 2: annealing > 1400 °C

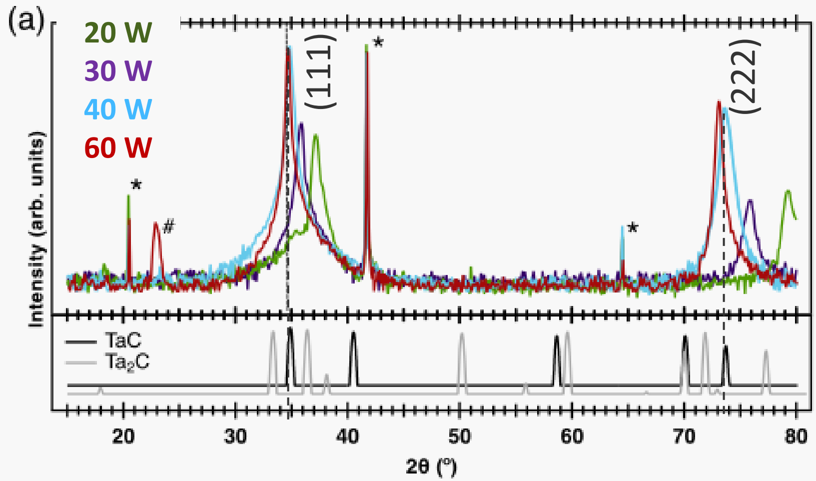
Improve crystal quality

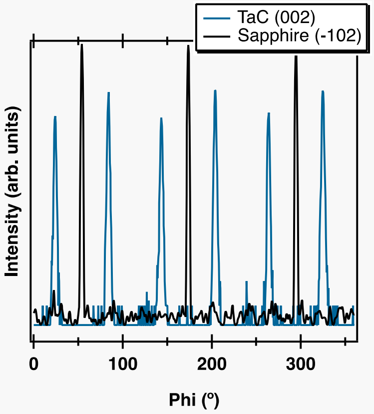


Step 3: epilayer growth

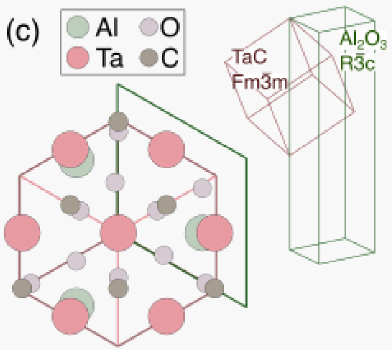
Grow LM AlGaN by MBE

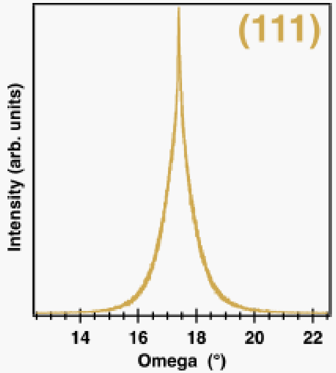
Sputter growth of TaC thin films on sapphire

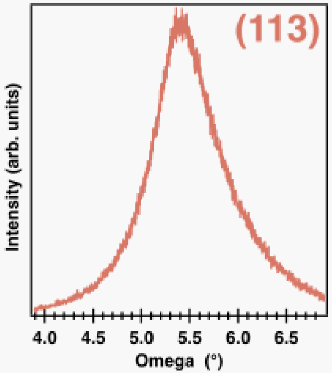




- Crystallinity improves with TaC target power
- Twins with slight site preference





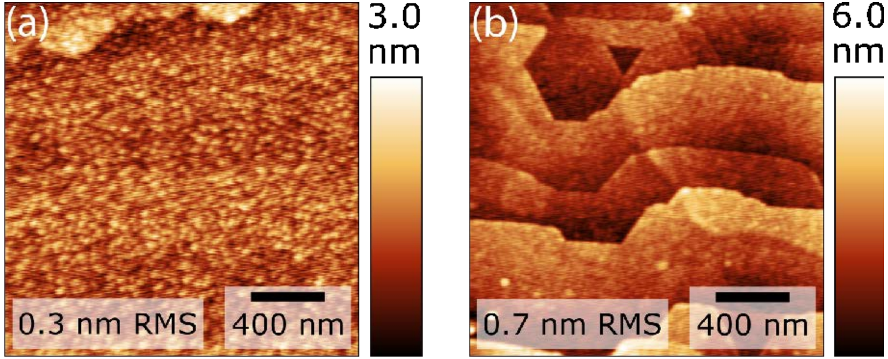


- In-plane relationship $\{11\bar{2}\}_{TaC} \parallel (10\bar{1}0)_{Al2O3}$
- Verify TaC presence and track structural quality via in plane (113) peak

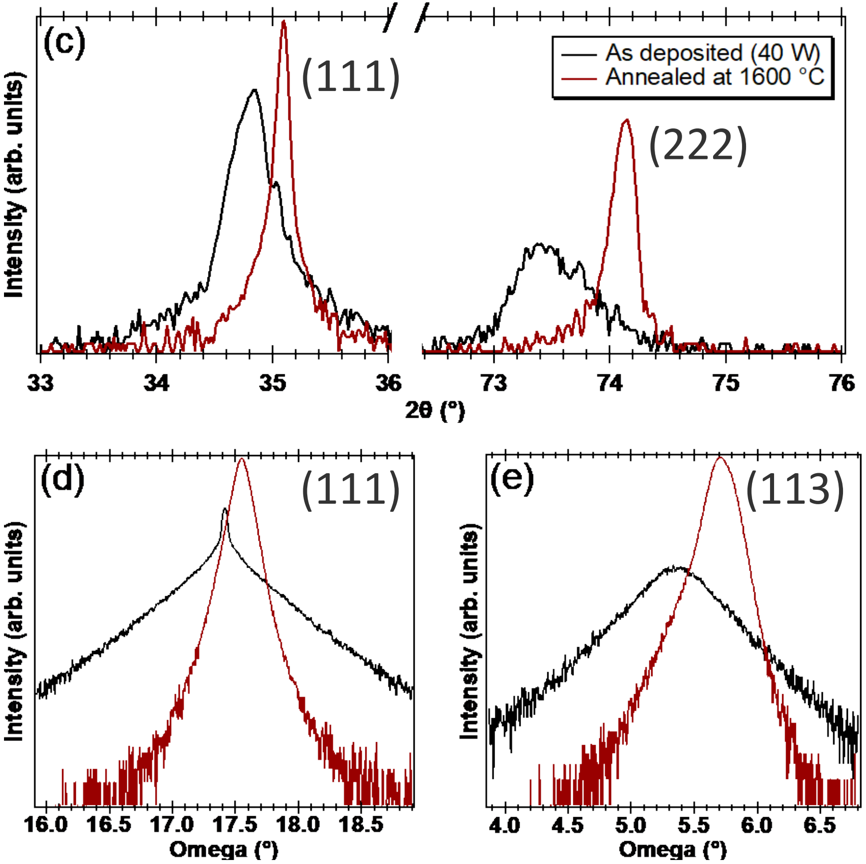
Roberts, et al – manuscript in submission (2024)

Engineering substrate layers

Annealing at 1600 ºC in a face-to-face configuration results in step-and-terrace surfaces and significantly improved crystallinity as measured by XRD

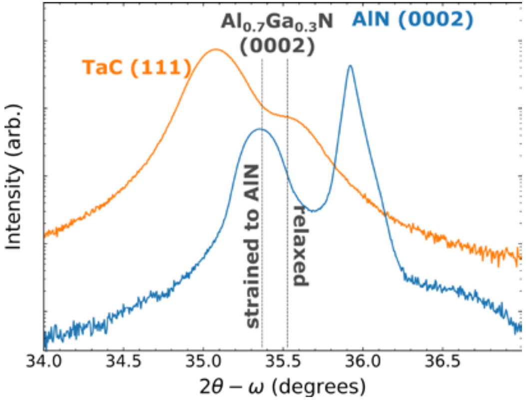


AFM of surface as deposited and after annealing



X-ray diffraction and rocking curves before and after annealing

Growth of AlGaN on TaC and analysis of interface



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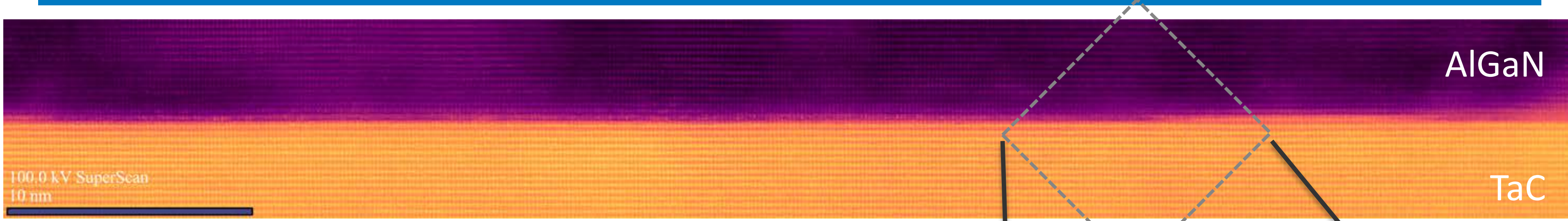
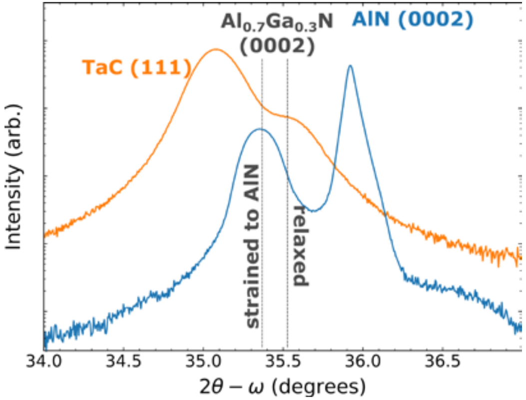
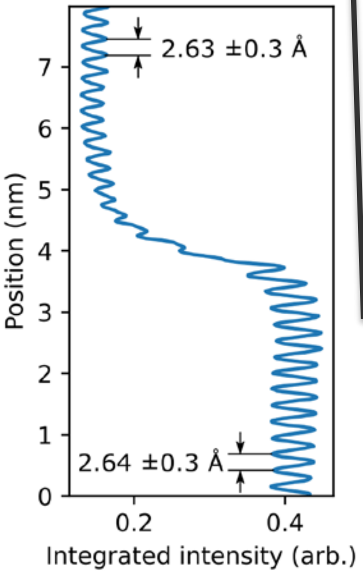
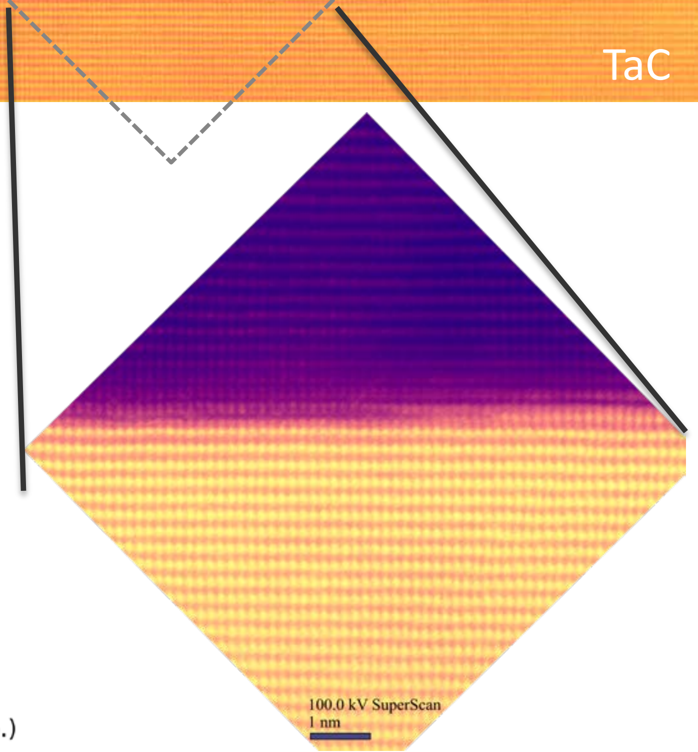


HAADF in collaboration with CNMS

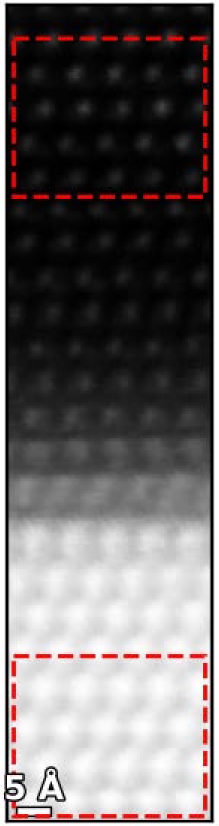






- Contrast variation indicates inhomogenous composition directly above the interface
- Some defects and stacking irregularity are observed
- However – fairly abrupt interface!

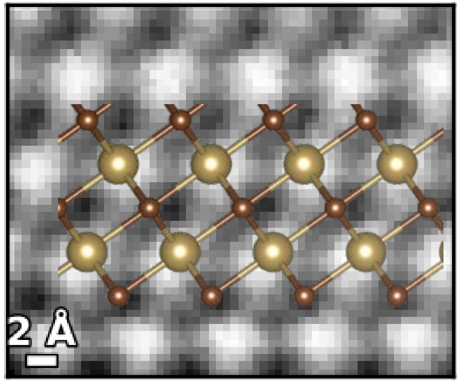
Clear metal polar wurtzite observed by atomic resolution STEM imaging



Metal and nitrogen positions are clearly visible by annular dark field

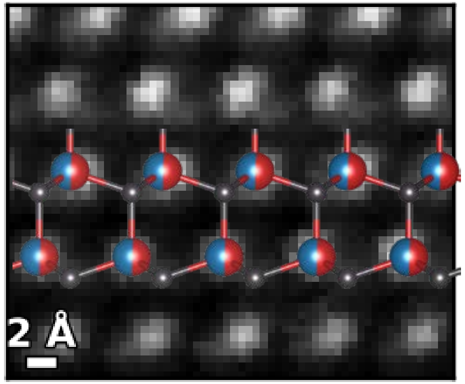
TaC rock salt structure clearly observed

TaC



$10\bar{1}$ zone axis

AlGaN

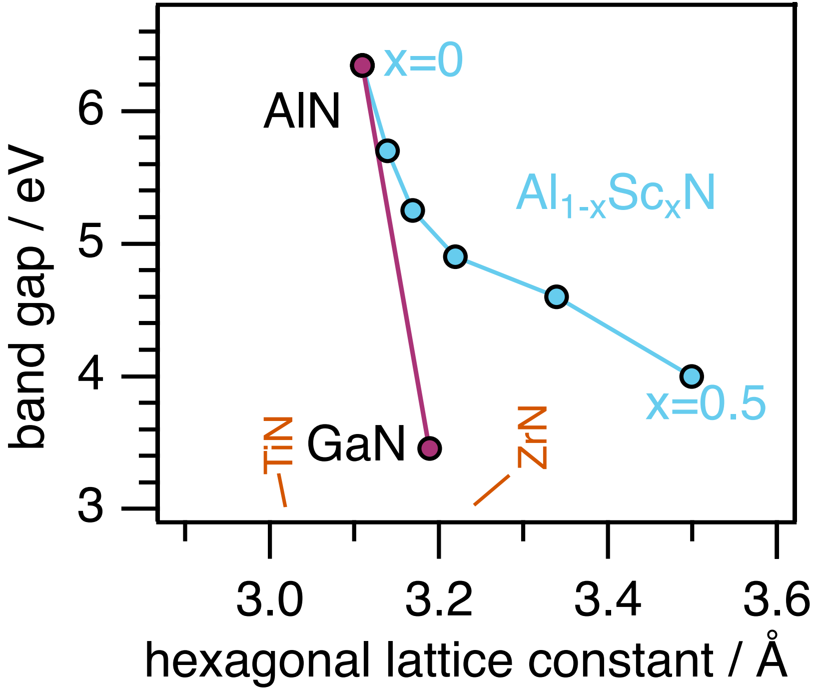


$11\bar{2}0$ zone axis

Substrates for other alloys

AlScN, AlGdN, etc

Virtual Substrates for Larger Lattice Constant Alloys



- Both carbides and nitrides are attractive for AlGaN, AlScN, and AlGdN alloys
- ZrN is appropriate for larger lattice constants but is difficult to stabilize – address with compositional grading

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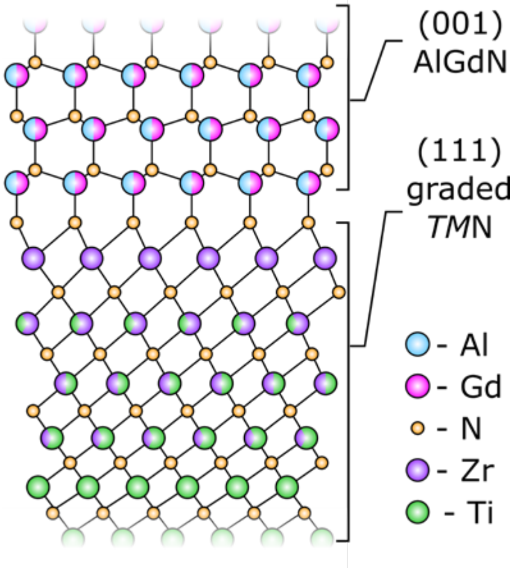

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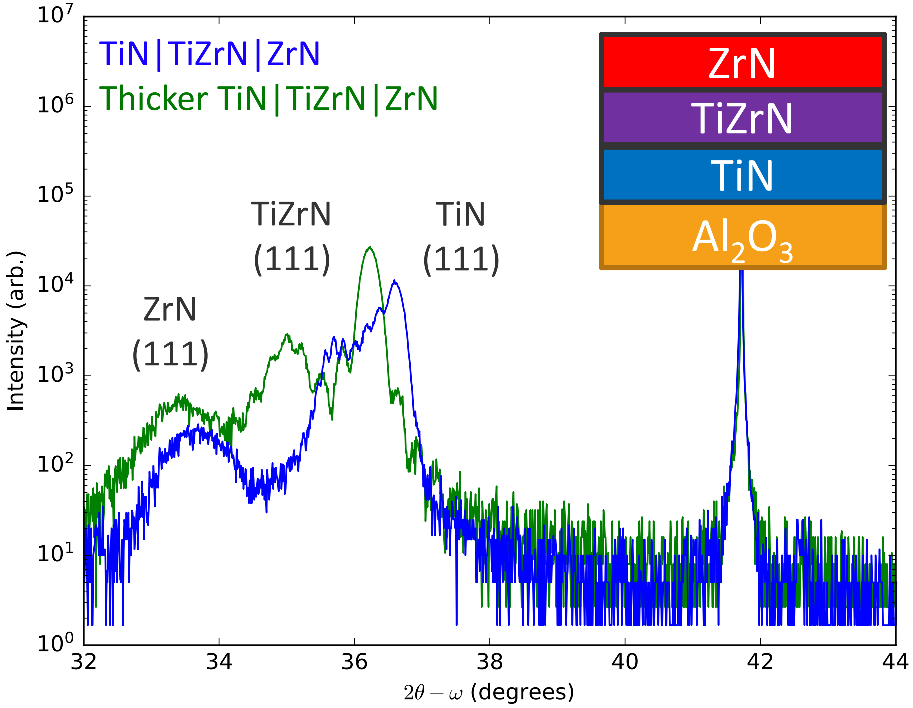
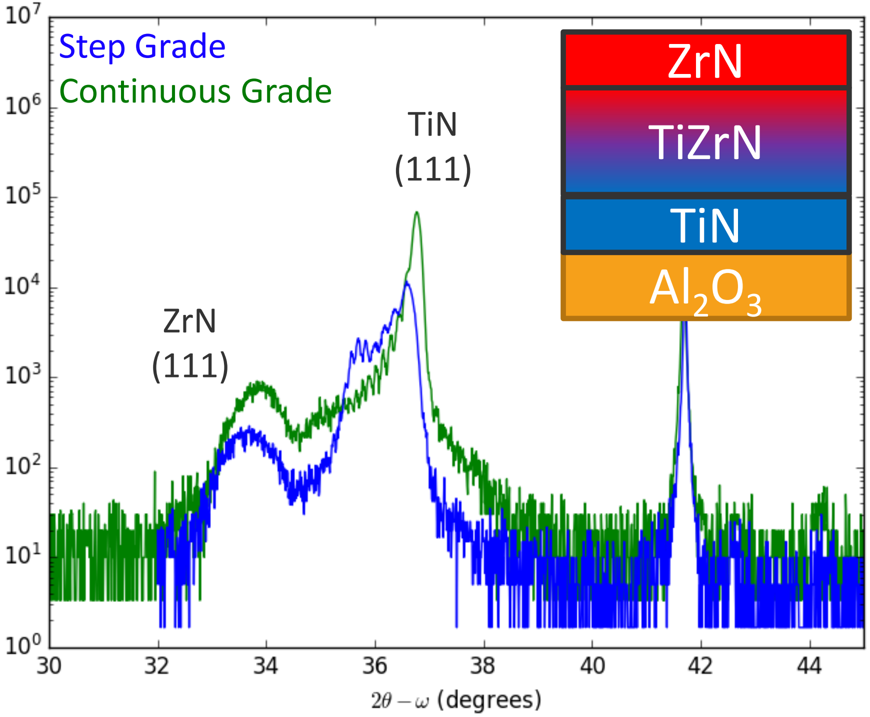
Graded transition metal nitride buffers by RF Sputtering

Step Grade

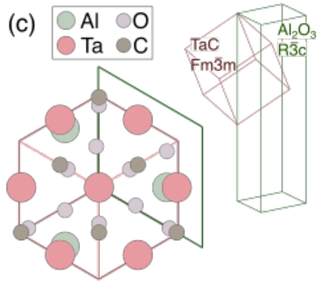


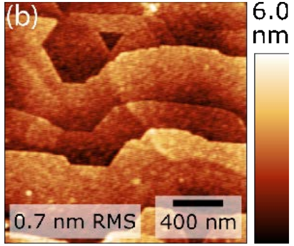
Continuous Grade

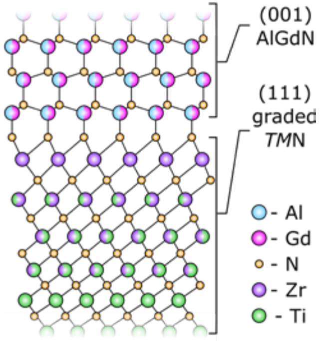


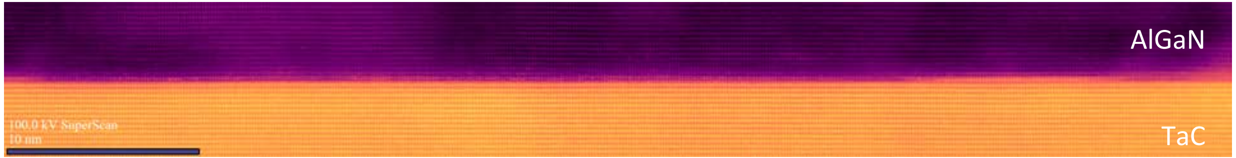
Conclusions – thin film virtual substrates can provide metallic lattice matching for Al-X-N

- TaC thin film virtual substrates were created by RF Sputtering
- Face-to-face annealing is effective at improving the crystallinity and surface morphology
- Rocksalt nitride compositional grades (step and continuous) have been demonstrated by RF Sputtering
- Proof of concept heteroepitaxy demonstrates the potential for low cost and scalable virtual substrates












Thank you!

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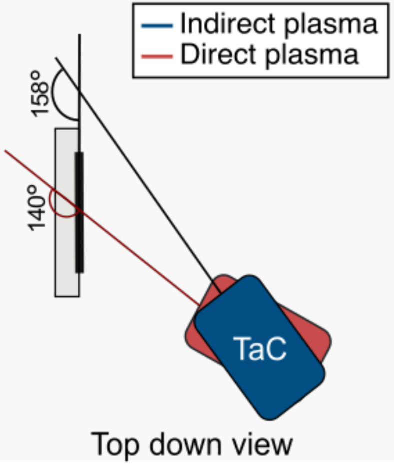
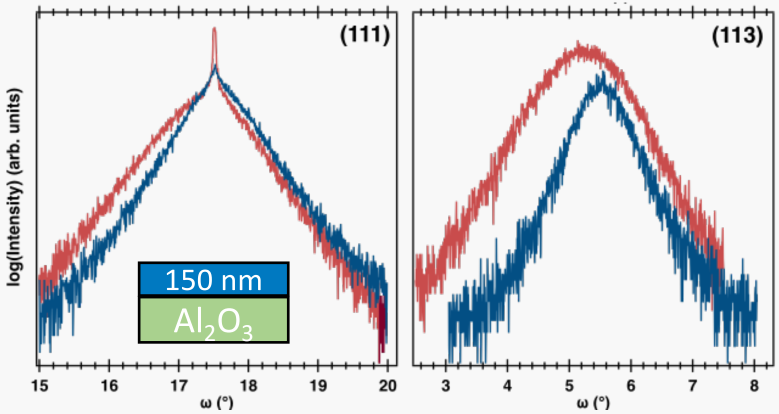
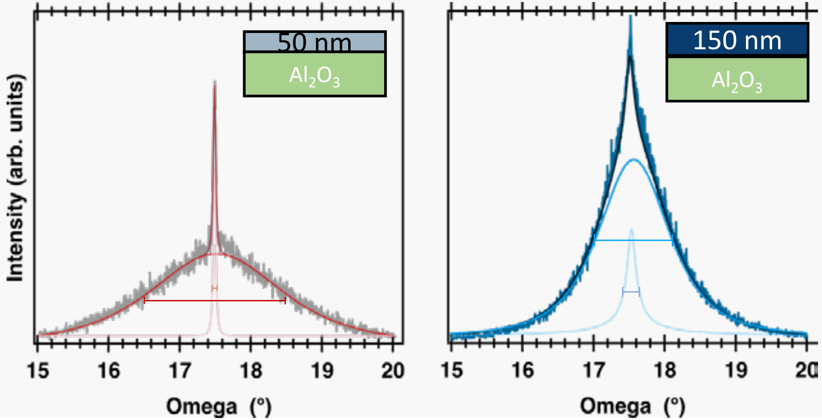
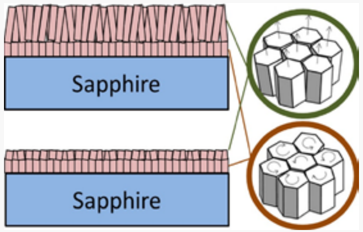
Effects of thickness and incident angle





Fewer in-plane defects in indirectly sputtered film

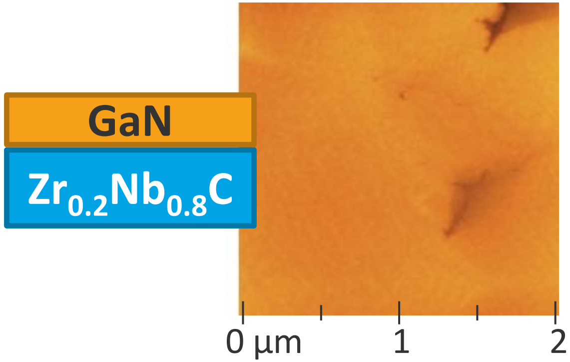


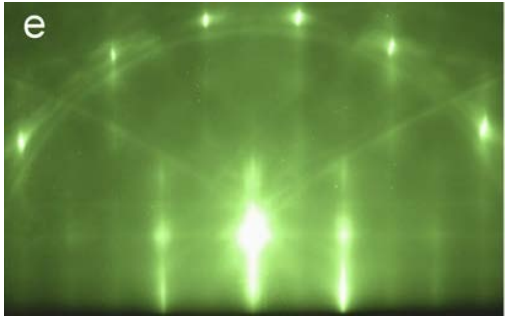


AlN on Sapphire
Miyake et al, J. Crys Growth 2016

Proposed solution

Surface AFM





Aizawa et al, J Crys Growth 2008

Previous literature

Inspired by Amano *et al* GaN studies – growth on $Zr_{0.2}Nb_{0.8}C$

Proposed work

- Transition metal carbides and nitrides
    - TaC (111) is lattice matched to $Al_{0.55}Ga_{0.45}N$
    - Compatible coefficient of thermal expansions
- Potential tunability via alloying