Awards Ceremony and Honorary Lecture
Room Town & Country A - Session HL-WeHL

Bunshah Award Honorary Lecture

Moderator: Dr. Ivan G. Petrov, University of Illinois at Urbana-Champaign, USA

6:05pm **HL-WeHL-2 R.F. Bunshah Award and ICMCTF Lecture Invited Talk: What TEM, XRD, STM, AFM, HIM, LEED, 3DATP, DSC, Nanoindentation, DFT, and MD Tell You About Functional Nanostructured Ceramics**, ***Lars Hultman***[1], Linköping University, Sweden **INVITED**

This presentation reviews strategies for characterizing diverse nanostructures that form in functional nitride thin films during vapor deposition intended to enhance mechanical and electronic properties. Material design is obtained by self-organization during surface- and bulk-driven segregations and phase transformation in metastable TiAlN, ZrAlN, HfAlN, TiSiN, MoVN, VWN, and InAlN alloy model systems, and analyzed by a suite of materials science tools. Density functional theory (DFT) calculations are employed to assess phase stability and decomposition from lattice mismatch and electronic band structure effects. The concept of age hardening is discussed for isostructural systems whereby spinodal decomposition is established for TiAlN by the formation of cubic-phase nm-size domains in a checker-board-pattern of TiN and AlN during annealing, as studied by XRD, TEM, atom probe tomography (APT) and differential scanning caloriometry (DSC). 2-D-nanolabyrinthine structuring in ZrAlN is obtained from the intergrowth of non-isostructural phases *c*-ZrN/*w*-AlN: {110}‖{11-20} interfaces. Focused-ion beam (FIB) is used to prepare cross-sectional TEM samples of TiN-based films with nanoindents to study plastic deformation from dislocation slip. Superhardening in TiN/Si_3N_4nanocomposites takes place due to Si segregation forming a few-monolayer-thick SiN_x tissue phase, which is a vacancy-stabilized cubic-SiN_x layer, as shown by STM, LEED, and annular-bright-field STEM.Si segregation is demonstrated in APT using ^{15}N isotopic substitution to resolve mass spectral overlap between Si and N. DFT is combined with molecular dynamics (MD) simulations to study growth of TiN with a competitionfor preferred crystallographic orientation (001) vs (111). High fluxes of low-energy (~20 eV) nitrogen ions control atomic layer roughening and yield low-temperature sputter epitaxy, as adatoms diffusing on an upper terrace require an additional energy (the Ehrlich barrier) to cross descending step edges. The barrier asymmetry at step edges leads to up-hill flux resulting in kinetic roughening.Step-flow growthof ductile inherently nanolaminated MAX phases like$Ti_3AlC_2$is confirmed by atom force microscopy (AFM) and helium ion microscopy (HIM). Scanning TEM/EDX elemental mapping reveals a new growth phenomenon - transmorphic heteroepitaxy – which takes place between CVD-grown AlN epilayer and SiC(0001) wafer substrates. The atomic chemical configuration transits over two atomic layers from SiC to AlN. The resulting AlN layer enables growth of high-quality thin GaN HEMT heterostructures.Finally, curved-lattice epitaxial growth of $In_xAl_{1-x}N$ core-shell nanospirals is presented.

[1] **R.F. Bunshah Awardee**

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