

Probing Growth-Induced Nanostructure Formation in Low-Energy Ion-Assisted Reactive Sputter Deposited Films

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Metastable transition-metal aluminum nitrides can develop complex nanostructures during reactive sputter deposition. Understanding their formation requires distinguishing atomic redistribution occurring at the growing surface from decomposition of an already formed metastable solid solution. Here, we examine $\text{Zr}_{1-x}\text{Al}_x\text{N}$ and $\text{Hf}_{1-x}\text{Al}_x\text{N}$ films deposited by ion-assisted reactive magnetron sputtering.

In $\text{Zr}_{1-x}\text{Al}_x\text{N}$ strong ZrN–AlN immiscibility drives segregation during growth, while chemical, interfacial and coherency-strain energies determine the resulting structure. For $0.2 \leq x \leq 0.4$, surface-mediated segregation produces a nanolabyrinthine arrangement of semi-coherent cubic ZrN- and wurtzite AlN-rich domains, from below 1 nm to ≈ 4 nm. Their length scale is governed by atomic mobility, revealing the coupling between thermodynamic driving forces and redistribution kinetics. At higher Al contents, the transition towards wurtzite changes the segregation pathway and reduces diffusion, demonstrating a crystal-structure dependence of nanostructure formation.

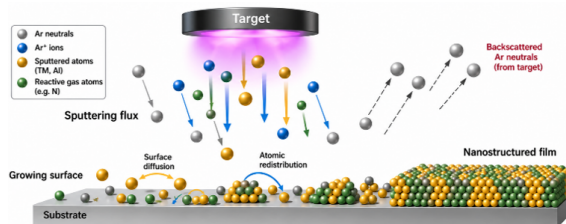


Figure 1: Schematic illustration of sputter deposition, surface-mediated atomic redistribution, and nanostructure development.

$\text{Hf}_{1-x}\text{Al}_x\text{N}$ reveals an additional growth-induced mechanism. Cubic films develop a three-dimensional compositional modulation of Hf- and Al-rich domains. X-ray diffraction and STEM reveal the superstructure,

while simulations show that energetic Ar neutrals backscattered from the Hf target can exceed the atomic displacement threshold and induce atomic rearrangements beneath the growth surface. Changes in substrate temperature and externally supplied low-energy ion flux produce comparatively small structural changes, highlighting the role of the arriving particle-energy distribution.

At these length scales, details matter apparently minor structural features can carry major mechanistic significance. Small differences in composition, local ordering or interface coherency can change the structural interpretation and the inferred formation mechanism. Resolving such features therefore requires complementary characterization across length scales rather than reliance on a single structural probe.

Together, these results show how mixing enthalpy, crystal structure, surface mobility and the energy distribution of the sputtered flux couple during growth to select the nanostructure of metastable transition-metal nitrides.

References

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