Experimental synthesis and atomic-scale characterization of metastable $TM_{1-x}Al_xN$, TM = Ti, V, Sc with emphasis on vacancy-mediated phase stability

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Metastable transition-metal aluminum nitrides ($TM_{1-x}Al_xN$, TM = Ti, V, Sc) represent a critical class of protective and functional coatings valued for their high hardness, superior thermal stability, and excellent oxidation resistance. While TiAlN and VAlN are well-established in industrial applications in their metastable cubic phase, ScAlN has recently attracted significant attention due to its outstanding piezoelectric properties in the wurtzite structure. Nevertheless, the fundamental mechanisms controlling the critical aluminum (or scandium) solubility limit and the role of point defects, particularly metal and nitrogen vacancies, in stabilizing or destabilizing these metastable solid solutions remain insufficiently understood.

Previous studies on reactive magnetron sputtering of TiAlN and VAlN have shown that substrate temperature, deposition rate, and residual stress influence the maximum Al solubility [1,2,3]. Building upon this foundation, the present work systematically investigates how deposition-induced vacancies (both on the metal and nitrogen sublattices) govern the stress state, phase stability, and critical solubility limit in $TM_{1-x}Al_xN$ systems, with special emphasis on ScAlN.

This work addresses key knowledge gaps in ScAlN research, particularly the limited understanding of vacancy formation, clustering, and their interaction with Al/Sc incorporation under non-equilibrium growth conditions. Vacancy concentrations will be tuned by varying ion energy, substrate bias, and nitrogen partial pressure, and their impact will be studied via subplantation mechanisms. Advanced atomic-scale characterization techniques will quantify vacancy populations, phase composition, interfacial strain, and defect evolution.

The obtained insights will advance the fundamental understanding of defect-engineered metastable nitrides and provide guidelines for tailoring next-generation high-performance ScAlN-based coatings with superior thermal stability and piezoelectric properties.

References:

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