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13-17 September 2021
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TRIB / Plasma - deposited protective and tribological coatings

Structure, stress and mechanical properties of Mo-Al-N sputter-deposited thin films: role of point defects

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Abstract content

In this work, the structural and mechanical properties of ternary Mo-Al-N alloys are investigated by combining thin film growth experiments and density functional theory (DFT) calculations. $Mo_{1-x}Al_xN_y$ thin films with various Al fractions ranging from x = 0 to 0.5 and nitrogen-to-metal ratio ranging from y = 0.78 to 1.38, were deposited by dc reactive magnetron cosputtering from elemental Mo and Al targets under $Ar+N_2$ plasma discharges. The elemental composition, mass density, crystal structure, residual stress state, and intrinsic (growth) stress were examined by WDS, XRR, XRD (including pole figure and $\sin^2\psi$ measurements), and real-time *in situ* wafer curvature. Nanoindentation tests were carried out to determine film hardness *H* and elastic modulus E_{IT}, while the shear elastic constant C_{44} was measured selectively by surface Brillouin light spectroscopy.

All deposited $Mo_{1-x}Al_xN_y$ films have a cubic rock-salt crystal structure and exhibit a fiber-texture with a [001] preferred orientation. The incorporation of Al is accompanied by a rise in nitrogen content from 44 to 58 at. %, resulting in a significant increase (2%) in the lattice parameter when x increases from 0 to 0.27. This trend is opposite to what DFT calculations predict for cubic defect-free stoichiometric $Mo_{1-x}Al_xN$ compounds and is attributed to variation in point defect concentration (nitrogen and metal vacancies) when Al substitutes for Mo. Increasing substrate temperature from 350 to 500 °C has a minimal effect on the structural properties and phase composition of the ternary alloys but concurs to an appreciable reduction of the compressive stress from −5 to −4 GPa.

A continuous increase and decrease in transverse sound velocity and mass density, respectively, lead to a moderate stiffening of the shear elastic constant from 130 to 144 GPa with increasing Al fraction up to x = 0.50, and a complex and nonmonotonous variation of *H* and E_{IT} is observed. The maximum hardness of ~33GPa is found for the $Mo_{0.81}Al_{0.19}N_{1.13}$ film, with nitrogen content close to the stoichiometric composition. The experimental findings are explained based on structural and elastic constant values computed from DFT for defect-free and metal- or nitrogen-deficient rock-salt MoAlN compounds [1].

Thanks/Acknowledgement

The authors acknowledge the financial support from the Scientific and Technical Research Council of Turkey (TÜBİTAK) for post-doctoral fellowship (Contract No. 1059B191800197) and the Austrian Science Fund (Project No. P30341-N36). The computational results presented have been achieved using the Vienna Scientific Cluster (VSC).

References

[1] F. Angay et al., JVST A 38, 053401 (2020)