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Cation and anion vacancies in cubic molybdenum nitride

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Epitaxial MoN_x layers deposited on MgO(001) by reactive magnetron sputtering in 20 mTorr N₂ at $T_s = 600-1000$ °C exhibit a cubic rock-salt type structure, a N-to-Mo ratio that decreases from $x = 1.25-0.69$ with increasing T_s , and a lattice constant that simultaneously decreases from 4.26-4.16 Å. A combination of composition, thickness, lattice-constant, and atomic area-density measurements indicate that the rock-salt structure contains both anion and cation vacancies, with the Mo site occupancy X_{Mo} decreasing from 0.89 ± 0.06 to 0.70 ± 0.04 while the N site occupancy X_{N} increases from 0.60 ± 0.04 to 0.88 ± 0.04 , as x increases from 0.69-1.25. Density functional calculations for over 200 cubic MoN_x configurations confirm the energetic stability of both cation and anion vacancies and predict X_{Mo} to decrease from 1.00 to 0.67 for $x = 0.54-1.50$, while X_{N} increases from 0.50 to 1.00 for $x = 0.50-1.36$. The simulations are in good agreement with experiments and indicate a preference for a 75% site occupancy on both sublattices for compositions near stoichiometry, with $X_{\text{Mo}} = 0.75$ for $x = 1.00-1.22$ and $X_{\text{N}} = 0.75$ for $x = 0.86-1.00$. Correspondingly, cubic stoichiometric MoN is most stable in the NbO structure.

Keywords: MoN; vacancies; transition metal nitrides; sputter deposition; reactive sputtering; thin films

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