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B.D. Ozsdolay, K. Balasubramanian, D. Gall

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Cation and anion vacancies in cubic molybdenum nitride

B. D. Ozsdolay, K. Balasubramanian, and D. Gall

Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA

Epitaxial MoN_x layers deposited on MgO(001) by reactive magnetron sputtering in 20 mTorr N_2 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_{Mo} = 0.75 for x = 1.00-1.22 and X_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