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First principles investigation into the phase stability and enhanced hardness of TiN-ScN and TiN-YN alloys[1] VIJAYA ADHIKARI, NATHAN SZYMANSKI, INDIRAS KHATRI, The University of Toledo, Toledo, OH, DANIEL GALL, Rensselaer Polytechnic Institute, Troy, NY, SANJAY KHARE, The University of Toledo, Toledo, OH — We study the phase stability, mechanical properties, and electronic structure of two quasi-binary ceramic systems, Ti1-xScxN and Ti1-xYxN; x=[0, 1], using first principles methods based on density functional theory, cluster expansion formalism, and Monte Carlo techniques. Owing to the similarity in ionic radii and electronegativities of their respective transition metals, strong exothermic mixing of TiN and ScN is predicted, with four ordered intermetallic phases lying on the convex hull: TiScN2, TiSc8N9, TiSc9N10, and Ti3Sc2N5 and the phase diagram reveals an upper consolute temperature of 660 K. Endothermic mixing with significant upward bowing in the formation energy at intermediate concentrations, with the consolute temperature of 7225 K is predicted from the phase diagram of Ti1-xYxN. TiN, ScN, and YN are found to display hardness values of 23.4, 25.1, and 20.6 GPa respectively. The intermetallic phase Ti3Sc2N5 is predicted to exhibit an exceptionally high hardness of 27.3 GPa. We attribute enhanced hardness to strong nitrogen p and metal d hybridization, being related to 3d eg occupation, and decreased tendency towards shearing, being related to minimal 3d t2g occupation. We suggest Ti1-xScxN alloys for implementation in hard coating applications.

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