TUNING STRUCTURE AND MECHANICAL PROPERTIES OF Ta-C COATINGS BY N-ALLOYING AND VACANCY POPULATION

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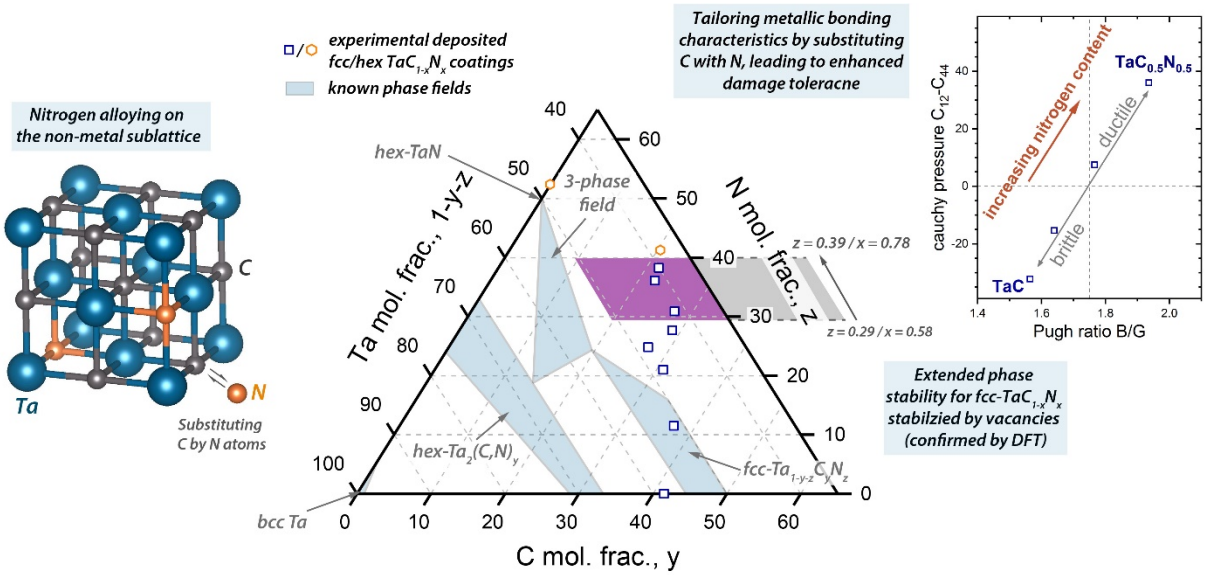
Transition metal carbides and nitrides are well established in various thin film applications due to their outstanding properties including extreme hardness, chemical inertness and highest melting temperatures. They exhibit a mixture of strong ionic, covalent, and metallic bonds but their application as structural components as well as thin films is limited by their poor fracture tolerance. Therefore, enhancing their fracture toughness, while retaining other thermo-mechanical properties is desirable for increasing the use of transition metal carbides in any application.



One conceptional approach is non-metal alloying, involving the exchange of C by N or vacancies on the non-metallic sublattice. Based on its high thermal stability as well as hardness Ta-C is used as a base system. Ta-C thin films were synthesized via non-reactive sputtering, while ternary Ta-C-N coatings have been deposited in N_2/Ar gas mixtures. Based on ab initio calculations, we could experimentally verify that structural defects, especially Ta vacancies, stabilize the preferred cubic structure for high N contents. We found single phase cubic structure up to a nitrogen content of about 68 % on the non-metallic sublattice. Furthermore, our DFT results predicted a softening of the films (confirmed by nanoindentation) and an increase of ductility—according to the Pugh's and Pettifor's criterion—with increasing N content. During uniaxial compression of superhard (43.3 GPa) 110-oriented $Ta_{0.47}C_{0.34}N_{0.19}$ pillars, we observed yielding at 16.9 GPa followed by plastic deformation where we identified {111} <01$\bar{1}$> as the most active slip system. From micro-

cantilever tests, we determined K_{IC} values of 2.9 compared to 1.8 MPa$\sqrt{m}$ for $Ta_{0.47}C_{0.34}N_{0.19}$ and $Ta_{0.55}C_{0.45}$ respectively, indicating that Ta-C-N exhibits indeed superior fracture tolerance compared to Ta-C.

This study gives a promising outlook on how mechanical properties can be tuned through alloying on the non-metal sublattice in transition metal carbides and nitrides based compounds.