EXPERIMENTAL AND THEORETICAL INVESTIGATIONS OF Ti-B-N-C FILMS

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Nanocomposite Ti-B-N-C coatings were deposited by magnetron sputtering of TiN and B_4C targets in the argon-nitrogen atmosphere at different nitrogen flow rates F_{N2}=0 (SPM-09), 2 (SPM-10), 4 (SPM-11), 7.5 (SPM-12) sccm. For the sake of comparison, TiN (SPM-13) and BCN (SPM-08) films were also deposited. To identify coating structures, X-ray diffraction and X-ray photoelectron spectroscopy investigations were carried out. The nanohardness (H) and elastic modulus (E) were determined through nanoindentation tests. The thickness of the coatings was determined with an optic profilometer. The thickness was 1.0, 0.6, 0.5 and 0.4 μm for SPM-09, SPM-10, SPM-11 and SPM-12, respectively, and 0.4 and 0.5 μm for SP-08 and SP-13, respectively.

The results of the investigations of the Ti-B-C-N, TiN and BCN films show that the Ti-B-C-N films are nanocomposite ones and represent the TiNC nanocrystallites (3.4-6.5 nm) embedded into the amorphous matrix that consists of amorphous boron nitride, a-BN, and amorphous carbon, a-C (nc-TiNC/a-BN/a-C). The films contain a small admixture of titanium oxides that are aggregated at the grain boundaries. The nanocomposite films deposited at high nitrogen flow rates were textured. An introduction of nitrogen prompts the formation of the TiNC nanocrystallites and the a-BN amorphous tissue, which, in turn, causes the improvement of the mechanical properties of the nanocomposite films. In Fig. 1 we show the values of H and E for the deposited films as functions of nanoindenter penetration. One can see that the best samples exhibited nanohardnes above 39 GPa.

First-principles molecular dynamics calculations with subsequent static relaxation of B1-TiN(001)-based heterostructures with one interfacial layer of B1-BN between slabs consisting of five TiN(001) planes were carried out to explain strength enhancement in the deposited nanocomposite films. It is shown that the BN interfacial layer forms an amorphous-like structure consisting of BN_3 units in the whole temperature range (0-1400 K). In Fig. 2, the calculated stress-strain curves for the TiN and TiN(001)/BN heterostructure are shown. Both the ideal shear and tensile strengths for TiN are higher than for the heterostructure. It follows that the observed strength enhancement in the deposited nanocomposite films should be ascribed mostly to the interfaces that play the role of barriers inhibiting dislocation motion.

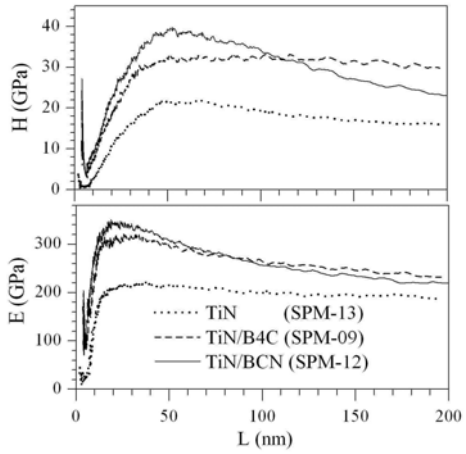

Fig. 1 Nanohardness (H) and elastic modulus (E) of the TiN and Ti-B-C-N films as functions of nanoindenter penetration

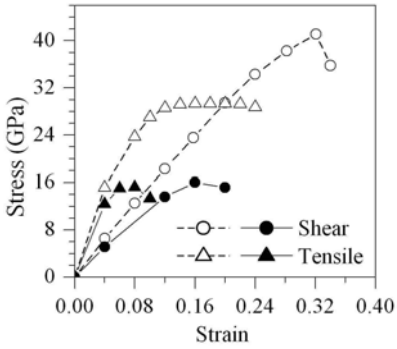

Fig.2 Stress-strain curves for the TiN (open symbols) and TiN(001)/BN (full symbols) structures under shear (010){001} strain and tensile [001] strain