INFLUENCE OF ALLOYING ELEMENTS ON THE MECHANICAL PROPERTIES, ESPECIALLY FRACTURE TOUGHNESS, OF THE WB_{2-Z} BASE SYSTEM

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Key Words: Thin films, Borides, Physical vapor deposition, Micromechanical testing, Fracture toughness

Transition metal diborides are an emerging class of thin film materials with promising properties ranging from ultra-low compressibility, high thermal stability, super hardness to superconductivity. These properties allow an application as protective coating in harsh environments. Our recent *ab initio* calculations suggest an attractive combination of both, high hardness and relatively high fracture toughness, for WB_2. This is enabled by a stabilization of the α-structure (space group 191, AlB_2-prototype, P6/mmm) over the intrinsic more stable ω-structure due to omnipresent point defects in physical vapor deposited coatings (*i.e.* boron and metal vacancies) [1]. However, those point defects in turn lower the thermal stability as the are affected by recovery events, leading to phase transformation into the ω-type. Further calculations point towards a stabilization of the α-type with the addition of Ta (which diboride is stabilized in the α-structure without the need of vacancies) at—compared to other transition metals investigated—low cost on ductility.

Within this study we deposited various $W_{1-x}M_xB_{2-z}$ solid solution coatings with different alloying element contents and examined them for mechanical properties and thermal stability. It was found for M=Ta that the hardness increases ~4 GPa (from 40.8±1.5 to 45.0±2.0 GPa) together with an improvement of the thermal stability (a change of the phase transformation temperature from ~800-1000 °C to over 1400 °C was observed) [2,3].

Besides these characteristics, in various applications a certain amount of damage tolerance (crack initiation and propagation) is required to prevent premature failure. To assess this behavior, we determined the fracture toughness of these coatings by performing micromechanical experiments by means of single cantilever bending tests within the framework of specifications given by Matoy *et al.* and Brinckmann *et al.* [4–6]. At the same time of the increase in hardness and thermal stability, we observe a decrease (in agreement with our DFT calculations) in fracture toughness (from 3.7±0.3 MPa√m for to 3.0±0.2 MPa√m) with the addition of tantalum up to a maximum content of 26 at% on the metal sublattice.

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