## MECHANICAL PROPERTIES AND FRACTURE BEHAVIOR OF TiB2+z THIN FILMS

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Hexagonal transition metal diborides are promising candidates for future protective coating materials as they exhibit an interesting mix of properties, i.e., high melting temperature, high hardness (~ 40 GPa), and excellent thermal stability. However, a significant drawback is their inherent brittleness, limiting possible long-term applications due to premature failure and subsequent environmental attacks. Within this study, we want to describe the fracture characteristics of physical vapor deposited titanium diboride thin films in more detail. We synthesized DC magnetron sputtered TiB<sub>2+z</sub> with a broad variation in boron contents (TiB<sub>2.07</sub> to TiB<sub>4.42</sub>) and investigated their elemental composition, morphology, and mechanical properties (hardness, Young's modulus, and fracture toughness). According to the literature, the boron-rich tissue phase is important regarding the mechanical properties of over-stochiometric TiB<sub>2+z</sub> thin films [1]. TEM investigations verified the presence of tissue phase and a decrease in grain size with increasing boron concentration. Furthermore, structural analysis confirmed the apparent correlation between the deposition pressure and a preferred texture within the TiB<sub>2+z</sub> thin films. To gain maximum hardness values (~40 GPa), a (0001) orientation (in growth direction) is essential, whereas for (1011) and (1000) oriented coatings, we observed a decrease in hardness of about 10 GPa. This strong anisotropic behavior (concerning active slip events) of hexagonal diborides was theoretically confirmed for ZrB<sub>2</sub> and TiB<sub>2</sub> and experimentally for WB<sub>2-z</sub> based thin films [2-4]. We conducted in-situ cantilever bending tests to determine the intrinsic fracture toughness - excluding possible substrate influences. These experiments revealed an almost linear decrease in fracture toughness from  $K_{IC}$  = 3.02 ± 0.13 MPa $\sqrt{m}$  for TiB<sub>2.43</sub> to  $K_{IC}$  = 2.51  $\pm$  0.14 MPa $\sqrt{m}$  for TiB<sub>4.42</sub>. We attribute this decrease, accompanied by a reduction in hardness, to the negative impact of excess boron (tissue phase).

In summary, our results highlight the impact of texture and morphological design on the mechanical properties of  $TiB_{2+z}$  based coatings. The 0001 texture emerged to be dominant concerning the hardness, whereas the constitution of the tissue phase mainly influences the fracture toughness.

References

[1] P. H. Mayrhofer, C. Mitterer, J. G. Wen, J. E. Greene, and I. Petrov, "Self-organized nanocolumnar structure in superhard TiB2 thin films," *Appl. Phys. Lett.*, vol. 86, no. 13, p. 131909, 2005, doi: 10.1063/1.1887824.

[2] B. Hunter *et al.,* "Investigations into the slip behavior of zirconium diboride," *J. Mater. Res.*, vol. 31, no. 18, pp. 2749–2756, 2016, doi: 10.1557/jmr.2016.201.

[3] S. Guo and H. Sun, "Superhardness Induced by Grain Boundary Vertical Sliding in (001)-textured ZrB 2 and TiB 2 Nano Films," *Acta Materialia*, vol. 218, p. 117212, 2021, doi: 10.1016/j.actamat.2021.117212.

[4] C. Fuger *et al.,* "Anisotropic super-hardness of hexagonal WB 2± z thin films," *Materials Research Letters*, vol. 10, no. 2, pp. 70–77, 2022, doi: 10.1080/21663831.2021.2021308.