Proceedings of the 6th International Conference on Mining, Material, and Metallurgical Engineering (MMME'19)
Lisbon, Portugal – August 15 - 17, 2019
DOI: 10.11159/mmme19.03

Transition Metal Diborides: Combining Computational and Experimental Materials Science

V. Moraes[1,2], Ch. Fuger[1], L. Zauner[2], R. Hahn[2], H. Bolvardi[3], P. Polcik[4], H. Riedl[1,2], and P.H. Mayrhofer[1,2]

[1] Christian Doppler Laboratory for Application Oriented Coating Development at the Institute of Materials Science and Technology, TU Wien, 1060 Vienna, Austria
[2] Institute of Materials Science and Technology, TU Wien, A-1060 Wien, Austria
[3] Oerlikon Balzers, Oerlikon Surface Solutions AG, 9496 Balzers, Liechtenstein
[4] Plansee Composite Materials GmbH, D-86983 Lechbruck am See, Germany

The increasing demand in various industrial applications, calls for a target-driven development of protective coatings with exceptional properties. Therefore, transition metal nitrides have been studied and developed extensively. However, the exploration of new protective coating systems is required to meet upcoming challenges not only in machining applications. Among the huge stoichiometric variety of borides, especially the diborides of transition metals (TMB_2) depict an interesting class for the use in protective thin films. Hereby, prominent representatives of this class (e.g., TiB_2, ReB_2, MgB_2, etc.) reveal excellent properties such as a high hardness, high melting point, great chemical inertness, high thermal or electrical conductivity or more extraordinary effects like superconductivity. Nevertheless, although their high potential and properties are well-known, the adaption to thin film solutions is rather limited in research history.

In the framework of this topic, we developed novel ternary diboride materials for the use in cutting and milling operations with focus on their thermal stability and mechanical properties. Therefore, instead of trial and error, we combine the fruitful approach of ab initio based density functional theory (DFT) calculations and well-established alloying concepts along with target-driven experiments. By using a pre-selection of materials for the best suitable candidates for selected concepts like age-hardening (e.g., coherent phase separation of supersaturated c-$Ti_{1-x}Al_xN$) or improvement of the phase stability (e.g. Yttria-stabilized ZrO_2), drawbacks of material properties such as brittleness can be tuned according to their demands in application. Thereby, the capturing of metastable phases achieved by utilizing physical vapour deposition techniques leads to entirely new material systems with exceptional properties.

Keywords: W_2B_{5-x} based diborides; multinary borides; mechanical properties; coherent phase separation;