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Ternary transition metal diborides – Next generation protective coating materials?

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Protective coatings for high-performance components – such as blades or powertrain systems in aero engines – constitute an important role for achieving further milestones with respect to carbon emission and environmental sustainability in general. Next to the well-established nitride-based coatings are boron containing systems an upcoming and highly promising class. Here, ternary transition metal diborides are relatively unexplored compared to their binary counterparts such as hard and inelastic TiB_2 or ZrB_2. In the design of novel ternary transition metal diborides diverse challenges arise, whereas the following are major factors: *(i)* composition-controlled crystallization in PVD based deposition techniques, *(ii)* limited fracture tolerance and brittle behaviour, as well as *(iii)* formation of non-adherent and volatile oxide scales. Within this study, we want address these specific challenges on various ternary model systems within group IV to VI transition metal diborides. The phase formation of two competing hexagonal structure types (α-AlB_2 vs ω-W_2B_{5-x}), with respect to target composition and ionization degree within the plasma, has been investigated for non-reactive DCMS, HiPIMS, as well as arc evaporation. In addition, different alloying concepts for enhancing the ductile character as well as oxidation resistance of these superhard ternary diborides will be discussed in detail (e.g. $W_{1-x}Ta_xB_2$ and others). To describe all these relations comprehensively, we correlated the synthesis parameters with structural and morphological evolution using XRD, HR-TEM, APT, as well as micro-mechanical testing methods. Furthermore, specific aspects have also been described by atomistic modelling (DFT).

Keywords
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