Formation of Planar Defects in Thin $V_{1-x}Mo_xB_{2-\Delta}$ Films

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Abstract. Thin films based on transition metal diborides (TMB_2) are widely studied due to their attractive physical properties. Combination of high-temperature stability and outstanding mechanical properties, such as high hardness and wear resistance, makes them suitable candidates for demanding applications in extreme conditions. In overstoichiometric $TMB_{2+\Delta}$ films, a self-organized nanocomposite microstructure consisting of TMB_2-P6/mmm hexagonal nanocolumns embedded in excess-boron tissue phase is formed, which leads to high hardness above 37 GPa [1–5]. However, the boron tissue phase forms a weak point in terms of oxidation resistance and brittle fracture. From this point of view, it seems promising to reduce the B/TM ratio and aim for understoichiometric $TMB_{2-\Delta}$ films, in order to obtain high hardness in combination with improved ductility and oxidation resistance [2,6–9]. In this work, we study ternary $V_{1-x}Mo_xB_{2-\Delta}$ coatings with different level of understoichiometry and discuss how the boron deficiency affects their structure and mechanical properties in the as deposited state, as well as after vacuum annealing up to 1300°C. We report on various types of planar defects identified by scanning transmission electron microscopy. In slightly understoichiometric $V_{0.58}Mo_{0.42}B_{1.9}$ system, anti-phase boundary defects were observed, which was accompanied by chemical separation of V and Mo. Accumulation of these defects led to formation of MoB-Cmcm orthorhombic phase in otherwise hexagonal VB_2-P6/mmm structure, with no apparent effect on mechanical properties. On the other hand, in case of highly understoichiometric $V_{0.37}Mo_{0.63}B_{1.2}$ coating, no chemical separation was observed. Here, annealing resulted in crystallization from amorphous state into orthorhombic Cmcm phase with high density of twin lamellae, which was accompanied by a significant hardening.

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