Influence of Boron Deficiency on Structural Stability of Thin $V_{1-x}W_xB_{2-\Delta}$ Films

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Abstract. Diborides of transition metals (TMB_2) are materials characterized by high hardness, wear resistance, electrical conductivity, and resistance to high temperatures, which makes them promising candidates for various thin film applications. Diboride films are usually prepared by physical vapor deposition (PVD) techniques, such as magnetron sputtering, which can lead to deposition of films with a wide range of chemical composition [1, 2]. Often observed excess or deficiency of boron leads to formation of various structural defects, which can have a significant effect on the mechanical properties [3-5]. In our work, we investigate the influence of boron understoichiometry (B/TM < 2) on structural stability of the ternary $V_{1-x}W_xB_{2-\Delta}$ system. Using density functional theory, we show that presence of boron vacancies destabilizes the system towards decomposition into hexagonal P6/mmm-VB_2 and orthorhombic Cmcm-$WB_{1\pm\delta}$ phase. Experimentally, we observed this structural separation in $V_{0.56}W_{0.44}B_{1.7}$ film prepared by magnetron sputtering and ex-situ annealed in vacuum at 1200°C. We present results of detailed structural analysis by high-resolution transition electron microscopy that revealed presence of anti-phase boundary defects which enable coherent transformation between the hexagonal and the orthorhombic phase.

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