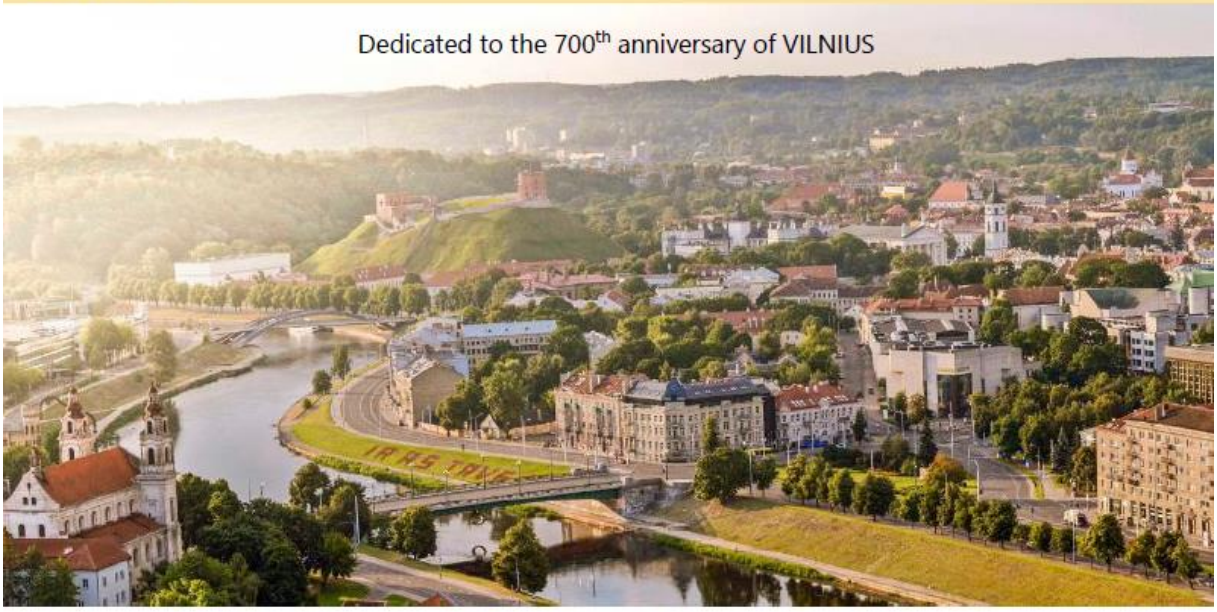
VILNIUS TECH
Faculty of Civil Engineering

The 14th International Conference

Modern Building Materials, Structures and Techniques

October 5-6, 2023, Vilnius
Lithuania

Dedicated to the 700th anniversary of VILNIUS



Conference Programme

The Conference is organised by the Faculty of Civil Engineering of VILNIUS TECH. The Conference will be held at the hotel Best Western Vilnius, Address: Konstitucijos pr. 14, Vilnius, 09308 Lithuania.

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Effect of transition metal doping on mechanical properties of tungsten diboride on the base of first-principles calculations and experimental investigations on magnetron sputtered films.

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The need to discover new materials is a scientific and industrial topic covering many different applications. Recent studies on superhard materials have shown that computational-based understanding and modeling serves as a reliable trend indicator which can be used to experimentally design new materials and their special properties. Transition metal borides are an extremely promising but, so far, poorly researched class of materials that can be used in a wide variety of applications, from wear resistant tools to nuclear fusion equipment. Unlike nitrides or carbides, the knowledge regarding these materials is not very large and requires further research, especially into compounds like ternary borides with improved ductility and increased crack resistance, correlated with great hardness.

In this work potentially superhard $W_{1-x}TM_xB_2$ polymorphs hP6-$P6_3$/mmc-WB_2 and hP3-P6/mmm, were thoroughly analysed with transition metal doping in the range of x=0-25%, within the framework of the first-principles density functional theory, from both a structural and a mechanical point of view (fig. 1). The obtained results were subsequently compared with the properties of material deposited by the magnetron sputtering method. All predicted structures are mechanically and thermodynamically stable. Theoretical calculations suggest a decrease in hardness *H* and fracture toughness K_{IC} of the hP6 phase with transition metal doping but no such effect on the hP3 phase. It was observed that an additional defect in the analysed structure significantly weakens the hP6 phase but strengthens the hP3 phase. The deposited films are characterized by greater than theoretical hardness (Hv = 42 GPa) for titanium but lower fracture toughness (K_{IC} = 3.2 MPa√m). The results of experiments show that not only is solid solution hardening responsible for strengthening the predicted new material but also the change in microstructure, the Hall–Petch effect and vacancies.

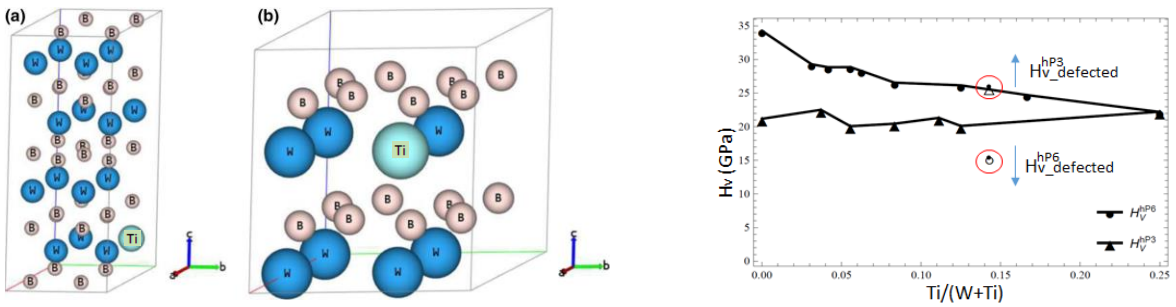

Fig. 1. Supercell with one W atom replaced by a Ti atom a,b), theoretical hardness in relation to amount of doping element in hP6-$P6_3$/mmc and hP3-P6/mmm WB_2 polymorphs c). Red circles means defected structure with WB_2 particle vacancy.

Acknowledgement

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