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# **Book of Abstracts**

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## Design of W-Al-B film properties: ab initio calculations and HiPIMS/DCMS combined deposition method

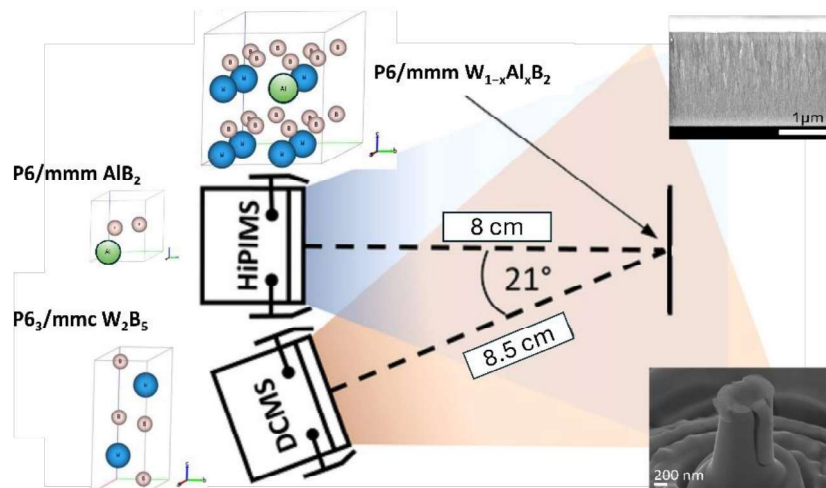
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### ABSTRACT

Tungsten diboride alloyed with additional metals provide an opportunity for obtaining exceptional mechanical, physical and chemical properties. We report a strategy for designing a superhard and incompressible ceramic films with increased toughness and lowered residual stresses ( $\sigma < -1$  GPa) deposited by high power impulse magnetron sputtering (HiPIMS) combined with direct current magnetron sputtering (DCMS). The use of a 20  $\mu$ s pulse allows to increase ionization of deposited material and in consequence quality of deposited films when DCMS provides the high deposition rate while maintaining exceptional mechanical properties even at a deposition temperature below 300 °C. The addition aluminium promote additional strengthening mechanisms in one material, leading to the improvement by two orders of magnitude of wear resistance compared to a undoped  $W_{1-x}Al_xB_2$ , yet, at even higher hardness and fracture toughness. The compression of micropillar shows that titanium addition change the type of fracture from cracking along slip plane to bulging on the top of pillar and next the crack initiation along column boundaries. The highest adhesion is obtained for 7% of aluminium in films and in all cases the wear of film has abrasive character.



The explanation of special features of presented coatings is not easy and need studies in different scales, starting from atomic scale. In this work potentially superhard polymorphs P6/mmm  $W_{1-x}Al_xB_2$  and P6<sub>3</sub>/mmc  $W_{1-x}Al_xB_2$ , were thoroughly analysed with aluminium 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.

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