High-entropy alloy inspired development of compositionally complex superhard (Hf,Ta,Ti,V,Zr)-B-N coatings

Andreas Kretschmer[1], Alexander Kirnbauer[1], Eduardo Pitthan[2], Daniel Primetzhofer[2], Kumar Yalamanchili[3], Helmut Rudigier[3,4], Paul Heinz Mayrhofer[1]

[1] Institute of Materials Science and Technology, TU Wien, Getreidemarkt 9, 1060 Vienna, Austria
[2] Department of Physics and Astronomy, Uppsala University, SE-75120 Uppsala, Sweden
[3] Oerlikon Balzers, Oerlikon Surface Solutions AG, Iramalli 18, 9496 Balzers, Liechtenstein
[4] OC Oerlikon Management AG, 8808 Pfäffikon SZ, Switzerland

andreas.kretschmer@tuwien.ac.at

Phase stability and mechanical properties of multimetal-boronnitride (Hf,Ta,Ti,V,Zr)-B-N are investigated by computational and experimental methods. Ab-initio calculations of (Hf,Ta,Ti,V,Zr)-B-N with different B:N ratios show a strong preference for the fcc NaCl-type structure over other structures (including the hcp AlB_2-type) up to a B:N ratio of 3.5. Reactive deposition of (Hf,Ta,Ti,V,Zr)-B-N thin films leads to the formation of fcc solid solution + X-ray-amorphous BN with a corresponding decrease in hardness from 32.5 (no B) to 16.7 GPa (18 at% B). Non-reactively sputtered (Hf,Ta,Ti,V,Zr)-B-N coatings are single-phase fcc solid solutions, up to the maximum B:N ratio of 1.12. All non-reactively sputtered multimetal-boronnitride coatings contain a high Zr metal-fraction and ~8 at% C. The single-phase coatings reach superhardness up to 46.3 GPa. Even after vacuum annealing to 1200 °C, the hardness of the coating with a B:N ratio of 1.03 is still 43.7 GPa, while that of $ZrN_{0.72}C_{0.28}$ decreased from 36.3 to 30.2 GPa. Our results demonstrate the importance of the deposition technique to allow for the formation of a single-phase fcc-(Hf,Ta,Ti,V,Zr)-B-N with exceptional properties.