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Mechanical properties and phase stability of an intriguing compound: Mo2BC

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Mo_2BC exhibits an orthorhombic crystal structure, which consists of layers of octahedral Mo_6C layers in a rocksalt structure, separated by face-sharing Mo_6B trigonal prisms. Here we report on ab initio calculations on Mo_2BC showing an enormously high stiffness (bulk modulus) exceeding that of typical protective coatings, such as TiN and TiB_2. This is combined with a relatively low shear modulus and a positive Cauchy pressure (c_{12}-c_{44}), indicating a highly stiff but moderately ductile material and thus inhibiting crack initiation and catastrophic failure. In order to test this hypothesis, thin films of Mo_2BC were synthesized on Al_2O_3(0001) at 850°C substrate temperature using DC magnetron sputtering from three single-element targets as well as a single compound target. The Young's modulus of ~460 GPa determined from nanoindentation measurements agreed very well with our calculations. Scanning probe imaging of a residual indent revealed significant pile-up around the indent and no crack formation was observed. This supports our hypothesis of moderate ductility and high stiffness of Mo_2BC. We attribute this seemingly contradictive behaviour to metallic interlayer bonding of stiff Mo-C and Mo-B bonds.
Thermal stability data of Mo_2BC thin films, assessed by means of differential scanning calorimetry, will also be presented. Initial results show that Mo_2BC is stable in Ar atmosphere up to at least 1000°C.

Keywords
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