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Synthesis of super-hard Mo–Al–Cr–N coatings: ab initio guided empirical approach

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The continuously growing demands for materials in machining industry are in need for further developments of multifunctional, high-performance coatings. Whereas TiN-, CrN-, and ZrN-based coatings are widely investigated, there is only limited information available about the MoN-based coatings. Although the high-temperature cubic phase γ-Mo2N possesses outstanding mechanical properties and therefore could be an excellent candidate for various high-demanding applications, at elevated temperatures it tends to react with the ambient oxygen forming volatile molybdenum oxides. In order to overcome this major limitation and to improve the oxidation resistance, the concept of alloying with Al and Cr was developed, since dense oxides (Al,Cr)O forming during tool operation inhibits further oxygen inward and molybdenum outward diffusion.
Based on our computational and experimental pre-studies we have aimed at synthesis of single-phase Mo2N-based super-hard coatings within the quaternary Mo–Al–Cr–N system. In contrast to several reports on the deterioration of mechanical properties of Mo2N by adding Cr [1] and Al [2], we have observed a sufficient hardness enhancement, also when adding Cr and Al in conjunction. Here, we show the importance of structural development along the quasi-binary tie lines Mo2N–XN, (X = Al, Cr), high Al- and low Cr-contents. The superhardness of 41.2 ± 2.9 GPa was obtained for Mo0.39Al0.52Cr0.09N. Moreover, increase of indentation hardness is not accompanied by increasing indentation modulus, which indicates the retaining ductility. Thus, the developed Mo2N-based super-hard coatings within the Mo–Al–Cr–N system have a high potential to be used as multi-purpose high-performance coatings.
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