Research Highlight

The hardest transition metal nitride predicted from Machine Learning

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The hardest transition metal nitride predicted from Machine Learning

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Materials that possess Vickers hardness (H_v) higher than 40 GPa are known as superhard materials, which have important applications in industry and scientific research. Commercially, there are only two types of superhard materials, i.e. diamond and cubic boron nitride (c-BN), which are widely used as cutting, polishing, drilling and coating materials. Although diamond has unrivaled hardness of 60–120 GPa, its applications in some circumstances, such as cutting ferrous materials, are limited due to very poor stability [1]. The main efforts in superhard materials research have been focused on the performance enhancements of existing superhard materials, and the design/synthesis of novel superhard phases. Previous studies indicate that nanotwinning can significantly enhance the hardness, toughness and stability of c-BN and diamond [2-4], and light-element (B, C, N and O) compounds with strong directional covalent bonds have potentially good mechanical properties and thermal stability [2].

For finding novel superhard phases, besides light-element compounds, transition metal light-element compounds with high valence electron density are also important candidates [5,6]. Such compounds have intrinsic high incompressibility and bulk modulus. Several hard transition nitrides (TMNs) have been predicted theoretically [7]. However, they have not been successfully synthesized. Among the synthesized TMNs, molybdenum and tungsten nitrides show the highest hardness [8]. Wang et al. [9] reported an ion-exchange reaction route to synthesize hard TMNs under pressures. The synthesized superconducting δ–MoN exhibits only the hardness of 30 GPa. Other novel tungsten nitrides with large elastic properties have also been predicted [10,11]. Unfortunately, they seem not superhard because of partial metallic components of chemical bonds [12]. Therefore, to find stable superhard TMNs is still a challenge.