Structure and Properties of $W_{1-x}Al_xB_{2-z}$ Coatings

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Abstract:

In the pursuit of advanced materials with exceptional properties, tungsten borides have attracted significant attention due to their remarkable hardness, thermal stability, and wear resistance. The crystallographic structure of such materials plays a pivotal role in determining their physical, mechanical, and thermal characteristics. Among these, aluminum-doped tungsten borides ($W_{1-x}Al_xB_{2-z}$) stand out, offering excellent mechanical and thermal properties. These materials show great promise for applications as protective coatings capable of maintaining stability at high temperatures.

To achieve the desired material structure, an innovative magnetron deposition method was employed, combining direct-current magnetron sputtering (DC) and High-Power Impulse Magnetron Sputtering (HiPIMS) techniques. The layer was deposited using two targets: AlB_2 (DC) and $WB_{2.5}$ (HiPIMS). An original method involving mass measurements and microscopic observations was applied to determine the density, which was subsequently used to calculate the thermal conductivity. The measured thermal conductivity values (5–8 W/(mK)) classify these materials as thermoelectric. Mechanical testing revealed very high hardness (~30 GPa for doping below 10% atomic aluminum) and a favorable plasticity index (H/E^*). As aluminum content increased in $W_{1-x}Al_xB_{2-z}$ layers, a slight reduction in density and hardness was observed, along with an increase in thermal conductivity.

Experimental results were compared with theoretical values obtained via DFT calculations. All $W_{1-x}Al_xB_{2-z}$ structures analyzed through DFT were found to be mechanically and thermally stable. The experimentally determined hardness values exceeded those predicted by DFT, underscoring the significant influence of aluminum doping.

This study highlights how deposition processes affect crystallinity, texture, and microstructural features, which in turn influence the material's mechanical and thermal properties. Optimization of deposition conditions and doping strategies enabled the development of $W_{1-x}Al_xB_{2-z}$—a promising material with potential industrial applications.

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