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Non-reactively sputtered ultra-high temperature Hf-C and Ta-C coatings

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Abstract

Transition metal carbides are known for their exceptional thermal stability and mechanical properties, notably governed by the carbon content and the prevalent vacancies on the non-metallic sublattice. However, when using reactive deposition techniques, the formation of amorphous C-containing phases is often observed. Here, we show that non-reactive magnetron sputtering of HfC_{0.89} or TaC_{0.97} targets lead to fully crystalline coatings. Their C content depends on the target-to-substrate alignment and globally increases from HfC_{0.66} to HfC_{0.76} and from TaC_{0.69} to TaC_{0.75} with increasing bias potential from floating to -100 V, respectively, when using a substrate temperature T_{sub} of 500 °C. Increasing T_{sub} to 700 °C leads to variations from TaC_{0.71} to TaC_{0.81}.

All HfC_y films are single-phase face-centered cubic, whereas the TaC_y films also contain small fractions of the hexagonal Ta₂C phase. The highest hardness and indentation modulus among all coatings studied is obtained for TaC_{0.75} with $H = 41.9 \pm 0.3$ GPa and $E = 466.8 \pm 15$ GPa.

Ab initio calculations predict an easy formation of vacancies on the C-sublattice, especially in

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