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Interface model and characterization for nanoscale ReB2/TaN multilayers with desired modulation period and ratios: First-principles and experimental investigations

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ReB_2/TaN multilayers were prepared using magnetron sputtering. Extensive measurements were employed to investigate the structure and mechanical properties of the multilayers. In order to explore the properties of TaN/ReB_2 multilayers or nanocomposite, we calculated the structure of TaN/ReB_2 system by density-functional theory (DFT).
The results demonstrated that the hardness of multilayers reaches a maximum value of 38.7 GPa at Λ=10 nm and t_{ReB2}:t_{TaN}=1:1 then decreases with Λ increases or t_{ReB2}:t_{TaN} decreases further. Almost all multilayers exhibit lower residual stress than the average value of monolithic ReB_2 and TaN coatings. We believe that periodic insertion of TaN into ReB_2 layers suppresses its grain growth, which releases stress build in the ReB_2 layers.The interfacial stability of a system can be measureed by its adsorption energy. The higher the interfacial energy is, the more stable the interfacial structure will be. The adsorption energy of B-Ta interface is higher than that of others. So the results showed that the B-Ta interface was the most stable interface. Microstructure evolutions in ReB_2/TaN multilayers are carefully investigated by differing modulation periods and modulation ratios. Clear coherent interface structure forms between epitaxial layers at the optimal modulation period of 10 nm, modulation ratio of 1:1. The fine nanocrystallities with small grain sizes are also kept stably in individual layers at the optimal modulation condition.

Keywords
ReB2/TaN multilayer
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density functional theory
interfacial stability
modulation