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Deposition Rates and Annealing Effects on the Growth of Nb Thin Film on Cu Substrate: Molecular Dynamic Simulation

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Abstract : To tackle the complexity of grasping atomic-scale structures and unraveling the factors affecting the development of thin films. In our work, we perform the deposition of Nb atoms on Cu substrates using the molecular dynamics simulation combined with the embedded atom method to describe the interaction between different atoms. We investigated the impact of varying deposition rates and thermal annealing processes on the microstructural, morphological, and mechanical characteristics of the deposited Nb film. Our findings reveal that Nb atom growth on the Cu substrate occurs in island mode, accompanied by the presence of nucleation phenomena during growth. On the other hand, mixing behavior was observed at the interface between the film and the substrate, where Nb penetration is initially limited to the first Cu layer, whereas Cu atoms diffuse until reaching the third layer in the Nb film. Furthermore, Nb exhibits a BCC structure, with a significant concentration observed at a rate of 5 atoms/ps, and annealing further amplifies these percentages. Deposition at different rates leads to distinct levels of compressive normal and biaxial stress.

Keywords : molecular dynamics, Nb thin film, structure and morphology, atomic penetration
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