

Interface structure between Nb thin film and MgO (112) substrate: A first-principles prediction

ABSTRACT

The crystal orientation of ceramic substrates is an important factor affecting the interface structure of metal/ceramic composite materials. However, there is little information about the interface composed of metal films and ceramic substrates with a high-index plane. In this work, we predicted the interface structure between a Nb film and a MgO (112) substrate by calculating the interface separation works of different interface models by using the first-principles calculation method. The results showed that the preferred growth direction is Nb [120], and that the value of the interface separation work is $0.35 \text{ eV}/\text{\AA}^2$. The lattice mismatch between the film and substrate is less than 3%, implying that a coherent interface type is highly realizable in Nb/MgO (112). Furthermore, we analyzed the interface structures of Nb/MgO (100), Nb/MgO (110), Nb/MgO (111), and Nb/MgO(112) and found that the unique atomic configuration of the MgO substrate is the main factor determining the preferred interface structure of Nb/MgO.