

The preferred growth orientation of Ti thin film on MgO(100) substrate

ABSTRACT

Understanding the preferred growth orientation of metal films is of great significance for optimizing film properties and preparing films with special structures. However, early works mainly focused on the preferred growth orientations of FCC and BCC metal films, the preferred growth orientation of HCP metal films and its formation mechanism are unclear. In this work, Ti film was deposited on MgO(100) substrate by magnetron sputtering at 523 K. The preferred growth orientation of Ti film and its formation mechanism were studied by experiment and first-principles calculation. XRD results found the preferred growth orientations of Ti film on MgO(100) substrate were Ti(001), Ti(100), and Ti(101), with Ti(001) being the most favored. First-principles calculation results showed the preferred growth orientation of the Ti film on the MgO(100) substrate was determined by a combination of interface separation work and lattice strain.