CRYSTALLOGRAPHIC ORIENTATION OF EPITAXIAL TRANSITION OBSERVED FOR NB (BCC) ON CU AND MGO (FCC) SINGLE-CRYSTALS

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Abstract

Niobium thin films were grown on (001) MgO (or Cu) single-crystal using a coaxial energetic deposition. The quality of the substrate surface and epitaxial Nb layers were investigated by the XRD and pole figure measurements. Depending on growth temperature, in-plane XRD show Kurdjumov-Sachs (KS) as well as Nishiyama-Wassermann (NW) epitaxial relationships for (110) and (001) Nb on (001) MgO. Calculation of the interface energy in rigid lattice models finds one KS and two NW minima. For the NW case the optimal atomic diameter ratio dbcc/dfcc=0.866 and 1.061, whereas for the KS case it is at dbcc/dfcc=0.919. Transitions of this type are usually induced by a change in the lattice parameter ratio resulting from a relaxation process in the early stage of the growth.

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