INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Special Seminar

Dr. S. Curiotto

Centre Interdisciplinaire de Nanoscience de Marseille
Aix-Marseille University, Marseille France

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Interfacial morphologies and orientation relationships between copper crystals and sapphire

The stability of an interface depends on its energy, which is often anisotropic, i.e. it depends on the crystallographic orientations of the phases at the interface. At equilibrium, the energy of an interface must be the lowest possible and therefore there will be a certain orientation relationship (OR) between the phases on the two sides of the interface.

As model system to study metal-oxide interfaces we have selected the system copper-sapphire. We have experimentally investigated the orientation relationships and the interfacial morphology of isolated copper particles equilibrated on sapphire (single crystal Al_2O_3) substrates with different surface orientations. Equilibration of the copper particles with the sapphire was achieved at 1253 K under an Ar-20%H_2 atmosphere either by solid-state dewetting or after liquid-state dewetting of copper films. Electron backscatter diffraction was used to determine the ORs between copper and sapphire: for the a-plane of sapphire, there is one preferred OR which is Cu(111)||Al_2O_3(2 -1-1 0) and Cu[1-10] within few degrees from Al_2O_3[0001]; for the m-plane of sapphire there are two preferred ORs: Cu(311)||Al_2O_3(10-10) and Cu[01-1] within few degrees of Al_2O_3[0001], and Cu(881)||Al_2O_3(10-10) and Cu[01-1] within few degrees from Al_2O_3[0001]. These three ORs are identical: indeed, when one (111) plane of a copper crystal is parallel to the (2-1-10) plane of sapphire, then either its (311) or (881) planes are parallel to the (10-10) plane of sapphire.

Scanning electron microscopy, atomic force microscopy and transmission electron microscopy were used to analyze the morphology of the copper-sapphire interface and of the sapphire surface in the vicinity of the triple line. The copper crystals tend to adopt their equilibrium shape, which significantly deviates from a simple truncated copper Wulff shape sitting on a flat sapphire surface. On the a-substrate, the interface remains flat but at a slightly lower level than the sapphire surface and small anisotropic ridges are formed at the triple line of the copper particles. The interface between the m-sapphire and the copper particles turns into a fully faceted hole and pronounced ridges surround the particles at the triple line. The role of the interfacial facets on the OR adopted by the copper crystals on the m-plane of sapphire will be discussed.