INTERFACES IN QUASICRYSTALLINE AND NANOCRYSTALLINE MATERIALS: 
QUASICRYSTALLINE AL – CU – FE AND AL – PD – MN ALLOYS 
AND 
NANOCRYSTALLINE TITANIUM, PALLADIUM AND THORIUM DIOXIDE

Abstract

The thesis is concerned with the structural characterisation of interfaces in quasicrystalline and nanocrystalline systems. Experimental work includes the synthesis of quasicrystalline Al-Cu-Fe and Al-Pd-Mn alloys and of thin-film metallic nanocrystalline titanium and palladium. These were characterised for the structure of interfaces along with nanocrystalline thorium dioxide by high-resolution transmission electron microscopy (HREM).

Al – Cu – Fe and Al – Pd – Mn are systems where stable icosahedral phases are found. In both systems, coexisting crystalline phases are found that are structurally related to the icosahedral quasicrystals. Two classes of interfaces have been studied in quasicrystals. In Al-Cu-Fe, quasicrystal – quasicrystal interfaces show a high degree of curvature with frequent, irregularly spaced ledges that are atomically flat with little disorder. For the second class of interfaces, similar interfacial structures have been observed at interfaces between the icosahedral phase and the related crystalline phase where the interfacial plane corresponds to the common symmetry axis shared by the two phases, in both Al – Cu – Fe and Al – Pd – Mn systems. The observed special features of grain boundaries and ledge interfaces are discussed in terms of co-operative alignment of common structural motifs and the orientation relation between the quasicrystalline and related crystalline phases.

Interfaces in metallic thin film titanium and palladium and ceramic thorium dioxide in powder and bulk form nanocrystalline systems have been studied. HREM images of interfaces are analysed for the state of order at the grain boundaries. The chief microstructural features seen in nanocrystalline metallic thin films are the bright contrast areas at triple line junctions, variability in lattice spacings and the presence of both ordered and disordered regions along the grain boundary. It is argued that the observed features of interface structures can be understood in terms of the disclination model of grain boundaries. The strain fields of disclinations can introduce disorder in the grain boundaries, curvature and also account for the disordered regions at triple line junctions. The lattice distortions in these materials have been quantified using the geometrical phase analysis technique. The results indicate that the atomic displacements are not localised to the interface region or isotropically distributed over the entire grain. Rather, there is a close relation between the presence of significant distortion in the grain and the presence of disorder at one or more interfaces of the grain with neighbouring grains. This again is as expected from the disclination model for grain boundaries and triple line junctions.