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ATOMIC SCALE SURFACE STRUCTURE OF AlPdMn QUASICRYSTAL: STUDY BY QUANTITATIVE PHOTOELECTRON DIFFRACTION

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One of the main developments in solid-state physics in the last two decades has been the discovery of quasicrystals (QCs) by Shechtman et al. (1984). Quasicrystal is a new form of the solid state which differs from the other two known forms, crystalline and amorphous, by possessing a new type of long-range translational order, quasiperiodicity, and a noncrystallographic orientational order associated with the classically forbidden fivefold (icosahedral), eightfold (octagonal), tenfold (decagonal), and 12-fold (dodecagonal) symmetry axes.

The surface structures of icosahedral and decagonal alloys have been examined previously with scanning tunneling microscopy (STM), low-energy electron diffraction (LEED) and X-ray photoelectron diffraction (XPD). In this paper, the technique of core-level XPD has been used to study the structure of the 5-fold symmetrical surface of an AlPdMn quasicrystal. The specific advantage of this technique is that it probes short-range order around the electron emitter, as it is seen from a certain types of atom in the crystal; this local diffraction method is complementary to LEED and x-ray diffraction, which are more sensitive to the long-range order.

The modeling of diffraction by means of the quasicrystal surface by means of clusters will be discussed. That includes the effect of depth and radius of cluster, the site of the cluster on the surface, and the effect of several parameters such as multiple scattering order, Rehr-Albers approximation order, phase shifts, inner potential, Debye temperature. The favored topmost surface layer was found and its relaxation was optimized. Detailed information about the favored surface structure will be presented and the origin of the main features in the XPD pattern will also be discussed.

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