Poster Presentation

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Phase transition and atomic structure of Cd6Tb 1/1 approximant to quasicrystal

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We present an in-situ temperature study of the atomic structure of the 1/1 Cd6Tb approximant to an icosahedral quasicrystal. It belongs to the 'Tsai' type family of quasicrystal and approximants whose archetype is the well-studied Cd-Yb system[1]. Its high temperature structure can be described as a bcc packing of a large Tsai atomic cluster, whose inner shell is a disordered tetrahedron at room temperature. As for most of the Cd6RE (RE=rare earth) approximant, the Cd6Tb phase undergoes a phase transition at 190 K to a phase of lower symmetry, resulting from an ordering of the inner tetrahedron[2]. Moreover, it has been shown that this phase undergoes a magnetic phase transition below 20 K, with an antiferromagnetic ordering of the Tb moment bearing atoms. It is thus particularly important to have a detailed structural study of this phase. We have carried out a systematic in situ measurement on a single grain from room temperature down to 40K on the crystal beam line located at the Soleil synchrotron. The structural phase transition is observed at about 190K. Using different attenuation, we have collected integrated intensity in a large dynamical range, leading to more than 60000 unique reflections in the C2/c monoclinic low temperature phase. The final wR2 values for room temperature and 40K are equal to 0.0726 and 0.0905 respectively. The resulting atomic structure will be compared to the well-studied approximant Zn6Sc, which is isostructural to Cd6Tb[3]. The ordering of the innermost tetrahedron leads to the distortion of the successive shells. The evolution of the high temperature phase, in particular just above Tc where pretransitional diffuse scattering is observed will be presented.

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