MS23-2-4 Phase transformation in a decagonal Al-Cu-Rh quasicrystal induced by phasons #MS23-2-4

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Abstract

Since the beginning of research on the structure of quasicrystals, the challenging question about the stability of these phases has not been answered with a clear answer [1]. The use of two competing mechanisms of structure stabilization (through entropy or energy minimization) in quasicrystals finds only partial theoretical and experimental verifications. In our presentation, we will present the results of the refinement of the Al-Cu-Rh decagonal structure model based on high-temperature data [2] using a new phason approach [3,4] and a generalized Penrose tiling (GPT) as a quasilattice [5]. Diffraction data were collected at temperatures 293 K and 1013-1223 K. A correlation was observed between lattice parameters and the maximum residual electron density was observed, indicating a phase transformation at around 1083-1153 K. At the same temperatures, the minima of values of moments, which model the phasonic flips, are observed, leading to the conclusion that the transition to a more stable phase is related to phason disorder.

The occurrence of the additional 5th atomic surface in GPT can be obtained by phasonic fluctuation in the ideal structure. In the consecutive refinement we observed that the atomic distribution of an 5th atomic surface correlates with the stability of a structure at the temperature of approximately 1153 K, which could indicate the influence of the phason disorder on the stabilization of the structure [6].

References

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