Poster Presentation

MS02.P09

High temperature structural study of decagonal Al-Cu-Rh quasicrystal.

P. Kuczera[1], W. Steurer[1]

[1]*Laboratory of Crystallography, ETH Zurich, Zurich, Switzerland*

The structure of d(ecagonal)-Al-Cu-Rh has been studied as a function of temperature by in-situ single-crystal X-ray diffraction in order to contribute to the discussion on energy or entropy stabilization of quasicrystals (QC) [1]. The experiments were performed at 293 K, 1223 K, 1153 K, 1083 K, and 1013 K. A common subset of 1460 unique reflections was used for the comparative structure refinements at each temperature. The results obtained for the HT structure refinements of d-Al-Cu-Rh QC seem to contradict a pure phasonic-entropy-based stabilization mechanism [2] for this QC. The trends observed for the ln(I(T1)/I(T2)) vs.|k⊥ |^2 plots indicate that the best on-average quasiperiodic order exists between 1083 K and 1153 K, however, what that actually means is unclear. It could indicate towards a small phasonic contribution to entropy, but such contribution is not seen in the structure refinements. A rough estimation of the hypothetic phason instability temperature shows that it would be kinetically inaccessible and thus the phase transition to a 12 Å low T structure (at ~800 K) is most likely not phason-driven. Except for the obvious increase in the amplitude of the thermal motion, no other significant structural changes, in particular no sources of additional phason-related configurational entropy, were found. All structures are refined to very similar R-values, which proves that the quality of the refinement at each temperature is the same. This suggests, that concerning the stability factors, some QCs could be similar to other HT complex intermetallic phases. The experimental results clearly show that at least the ~4 Å structure of d-Al-Cu-Rh is a HT phase therefore entropy plays an important role in its stabilisation mechanism lowering the free energy. However, the main source of this entropy is probably not related to phason flips, but rather to lattice vibrations, occupational disorder unrelated to phason flips like split positions along the periodic axis.

[1] *Kuczera P., Wolny J., Steurer W., (2014) Acta. Crtst. B70, doi:10.1107/S2052520613032575,* ***[2]*** *Henley, C. L. (1988) J. Phys. A Math. Gen. 21, 1649–1677*

Keywords: high-temperature structure, decagonal quasicrystal, stabilization mechanism