High-temperature structural studies of d-AlCuRh – phasonic stabilization

R. Strzałka, I. Bugański, J. Wolny

Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland

strzalka@fis.agh.edu.pl

We revisited X-ray diffraction data of decagonal Al-Cu-Rh system collected previously by Kuczera *et al.* [1] at room temperature and at 1013-1223 K. From [1] it is known, that the best quasiperiodic ordering exists most probably between 1083 and 1153 K. The stability was proven to be most likely not phason-driven entropy lowering.

In our recent studies, we tested an application of the new correction for phasons, based on the statistical approach. It was shown [2,3], that phason flips significantly change the shape of the average unit cell, and therefore influence the structure factor, and thus the diffraction diagram. These changes in the shape of the AUC can be handled analytically. During the structure refinement, the new correction for phasons gives an extra parameter to fit. The procedure was recently applied to room-temperature d-AlCuRh data [4].

We performed a series of structure refinements including a new correction term for phasons alongside the standard perp-space Debye-Waller factor for 5 sets of X-ray diffraction data at 293, 1013, 1083, 1153, and 1223 K. In the case of every dataset, we were able to achieve better *R*-factor values as compared to original results reported in [1]. As a result, phasonic ADPs were refined alongside the flip probability (measuring the phasonic contribution within the new approach), which shows a distinct minimum in the temperature plot (Figure 1). This can lead to a conclusion, that the amount of phasons is minimal at around 1153 K, which is also a temperature of maximal stability of the quasicrystal.

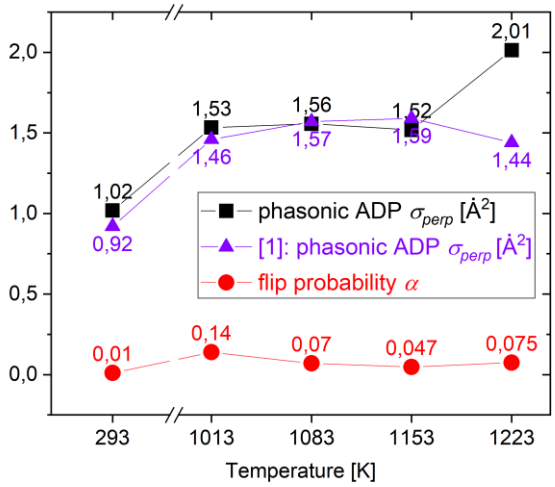

Figure 1. Phasonic ADPs (new and from [1]) and flip probability from the refinement *vs.* temperature.

[1] P. Kuczera, J. Wolny, W. Steurer, *Acta Cryst. B* 70 (2014) 306-314.

[2] J. Wolny, I. Buganski, P. Kuczera, R. Strzalka, *J. Appl. Cryst.* **49** (2016) 2106-2115.

[3] R. Strzałka, I. Bugański, J. Śmietańska, J. Wolny, *Arch. Metall. Mater.* **65** (2020) 291-294.

[4] I. Bugański, R. Strzałka, J. Wolny, *Acta Cryst. A* **75** (2019) 352-361.

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