In search of new magnetic quasicrystal approximants: flux–grown single crystals of monoclinic C2/m Al-Fe, Al-Fe-Cu, and Al-Fe-Cu-Si phases

Bardziński PJ[1,2*], Weselski M[1], Asimow PD[2], Hu J[2]

*lead presenter: piotr.bardzinski@uwr.edu.pl
1Faculty of Chemistry, University of Wrocław, Wrocław, Poland
2 Division of Geological and Planetary Sciences, Caltech, Pasadena, USA

Quasicrystals, which lack translational symmetry and hence can express forbidden rotational symmetries at macroscopic scale, are typically surrounded in composition space by nearby crystalline counterparts, known as approximants. These phases may contain the same clusters as the quasicrystal, with forbidden rotational symmetry at the atomic scale, but the clusters in the approximants are arranged in periodic crystal structures. In materials with such structure, one may expect potentially promising physical properties, such as exotic magnetic order or electronic transport [1]. As shown by Steurer [2], a monoclinic lattice can be linked to the decagonal quasicrystal by a group-subgroup relation. Several studies have identified intermetallic phases that crystallize in the monoclinic *C2/m* space group with nominal stoichiometry of $Al_{13}TM_4$or $Al_{76.5}TM_{23.5}$. where *TM* refers to one or more transition metals. Compounds considered to be quasicrystal approximants with this structure include $Al_{81.4}Cr_{3.3}Fe_{15.3}$ [3], $Al_{76.5}Ru_{23.5}$, $Al_{76.5}Ru_{20.0}Ni_{3.5}$ and $Al_{76.5}Ru_{17.6}Ni_{5.9}$ [4].

In the current study we report successful flux-growth of monoclinic single crystals of $Al_{76}Fe_{23}$, $Al_{74.2}Fe_{21.5}Cu_{4.3}$, $Al_{70}Fe_{27}Cu_3$and $Al_{64}Fe_{24}Cu_9Si_9$ with platelet morphology. Our experimental set up involves a centrifuging, decanting, corundum Canfield-type crucible held above the melting temperature of Al-flux, followed by quenching in room temperature water. Each of the four synthesized compositions corresponds to different starting conditions of the flux-growth process. Phases with stoichiometry matching the flux-grown monocrystals were identified by Energy-dispersive and wavelength-dispersive X-ray spectroscopy in rapidly solidified and equilibrated alloys. Electron Backscatter Diffraction reveals the presence of a ten-fold axis, characteristic of the decagonal quasicrystalline phase, in the rapidly solidified alloy phases. However, single crystal X-ray diffraction showed that the corresponding monocrystals always crystallized in the *C2/m* space group. Hence the flux-grown single crystals are approximants of the dodecahedral quasicrystals formed by rapid quenching. This might suggest that the decagonal phase is metastable and undergoes a quasicrystal–approximant transition during either the of flux-growth process or the decanting step. By contrast, we found that a paramagnetic approximant phase $Al_{71}Fe_9Cu_{20}$ transforms during heat treatment into an apparently stable $Al_{70.5}Fe_{24.0}Cu_{5.5}$ decagonal phase, which was found to be weakly ferrimagnetic at room temperature.

References

[1] Goldman, A. I. (2014). Magnetism in icosahedral quasicrystals: current status and open questions. *Science and technology of advanced materials*, *15*(4), 044801.
[2] Steurer, w., Twenty years of structure research on quasicrystals. Part I. Pentagonal, octagonal, decagonal and dodecagonal quasicrystals Z. Kristallogr. 219 (2004) 391–446
[3] Demange, V., Ghanbaja, J., Beeli, C., Machizaud, F., Dubois, J. M. (2004). Study of decagonal approximant and γ-brass-type compounds in Al–Cr–Fe thin films. *Journal of materials research*, *19*(8), 2285-2297.
[4] Murao, R., Genba, M., Sugiyama, K., Sun, W. (2011). The Structure of an Al-Ni-Ru Monoclinic Phase Al_{13} (Ru, Ni) $_4$. *Materials transactions*, *52*(7), 1344-1348.

The research described was funded by the National Science Centre, Poland (NCN) within the research grant No. 2020/36/C/ST5/00007.