Neutron diffraction study on the Pd-Ga-Tb 2/1 quasicrystal approximant

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Quasicrystal is a substance with long-range quasiperiodic atomic arrangement, nonetheless, with the rotational symmetry that is prohibited in the periodic crystals, such as the five-fold symmetry. The quasicrystal is, therefore, different from periodic crystals and random glasses, and now is regarded as the third form of solids. There is a class of crystals, called " approximants ", in which the high-symmetry (such as icosahedral) atomic clusters, identical to those in the quasicrystals, form periodic array, and thus being approximation of the quasicrystalline structure. The degree of approximation is expressed by the fractional numbers, such as 1/1 and 2/1. The 1/1 approximant is the lowest order approximation, in which the atomic clusters form a bcc cubic lattice. The 2/1 approximant has a larger unit cell, becoming a better approximation to the quasicrystal. As the fractional number becomes the irrational golden ratio $\tau \sim 1.618...$, the unit cell becomes infinitely large, i.e. quasicrystal.

Recently, for the first time we have determined magnetic structure of the antiferromagnetic 1/1 Au-Al-Tb approximant using ECHIDNA [1], which turns out to be a very intriguing non-collinear and non-coplanar whirling order. Quite recently, one of the proposers further found a magnetic 2/1 approximant in the Ga-Pd-Tb system, which orders antiferromagnetically at 5.8 K [2]. This is definitely the first 2/1 approximant that shows antiferromagnetic long-range order, which excites us enough to perform this neutron powder diffraction study.

A polycrystalline alloy of the Pd-Ga-Tb 2/1 approximant was prepared by arc melting with high purity ($>$ 99.9 wt%) Pd, Ga and Tb elements. The neutron powder diffraction experiment has been performed using the high-resolution powder diffractometer ECHIDNA installed at the OPAL reactor, Australian Nuclear Science and Technology Organisation [3]. For most of the magnetic diffraction measurement, neutrons with $\lambda = 2.4395$ Å was selected using the Ge 311 reflections, whereas for the structure analysis, to obtain reflections in a wide Q-range, we select $\lambda = 1.622$ Å using the Ge 335 reflections. The sample was set in the $\phi 6$ mm vanadium sample can, and then set to the cold head of the closed cycle ^{4}He refrigerator with the base temperature 3.5 K.

Figure shows the overall diffractograms at various temperatures ranging from the base ($\simeq$ 3.5 K) to the paramagnetic temperature 7 K. One can clearly see the development of sharp magnetic reflections below 5 K. They are the clear indication of magnetic long-range order in this 2/1 approximant. We further note that the magnetic reflection appearing at $2\theta \simeq 21.9$ degrees is relatively weak, compared to that observed in the Au-Al-Tb 1/1 approximant [1]. On the other hand, quite a few magnetic reflections can be seen in the Pd-Ga-Tb 2/1 approximant, number of which is much larger than that in the Au-Al-Tb 1/1 approximant. These results suggest that the magnetic structure would be much more complicated in the Pd-Ga-Tb 2/1 approximant, and is of significant interest in view of larger unit cell of the 2/1 approximant. The magnetic structure analysis using the representation analysis is in progress.

[1] T. J. Sato *et al.* (submitted); [2] Y. -G. So *et al.* (in preparation); [3] M. Avdeev and J. R. Hester, J. Appl. Crystallogr. 51, 1597 (2018).

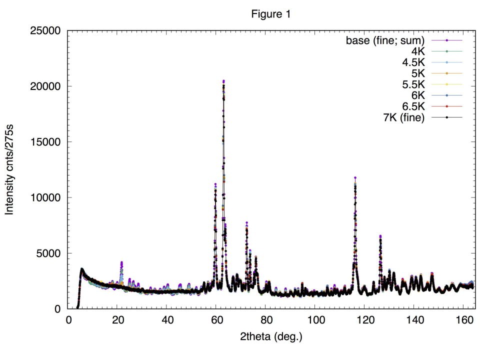

Fig. 1. Neutron diffraction patterns obtained in the temperature range $4 < T < 7$ K at ECHIDNA.