

Structure Analysis of P-type Icosahedral Zn-Mg-Ho Quasicrystal

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Since the first discovery of icosahedral quasicrystals (i-QCs) in 1984 [1], structure determination of these exotic materials remains a challenging problem. The p-Zn₇₅Mg₁₆Ho₉ belongs to a series of i-QCs known as p-Zn-Mg-R (R = rare earth elements) that was found in 2002 [2]. It is known that three large occupation domains (ODs, or atomic surfaces) in a unit cell characterize its six-dimensional (6D) structure by an x-ray diffraction study [3]. In addition, a triacontahedral cluster that is considered as an extended icosahedral cluster of Bergman type has been identified as one of the fundamental building units for the structure description [3]. Although, the 3D structure can be understood as an aperiodic arrangement of such triacontahedral clusters, its detailed atomic structure is still undetermined, since p-Zn₇₅Mg₁₆Ho₉ is a ternary alloy and the location of the lightest element, Mg, is not easy to determine by x-ray diffraction. In order to obtain complementary structural information to x-ray diffraction technique for determining a structure model of the p-Zn₇₅Mg₁₆Ho₉, we have performed a neutron scattering experiment on this i-QC.

The neutron four-circled diffractometer FONDER installed by Tohoku University at the beam line T2-2, JRR-3M in JAERI was used for the experiment. The neutron wave length of 1.24 Å (Ge 311 monochromator) was used. The volume of single crystal sample used was 66 mm³. The intensity data of selected strong 544 Bragg reflections ($2\theta < 150^\circ$) were measured and 324 reflections were observed at room temperature.

Using the present neutron diffraction data, together with the structural phases from a model by x-ray diffraction, nuclear densities in the 6D space have been reconstructed (figure 1). The reconstructed nuclear densities exhibit ODs in which contribution from Mg atoms is enhanced compared with the electron densities that were obtained by x-ray diffraction data [3]. In particular, an extra small OD, which was not recognized in the previous study, was found as indicated by the ellipse in Fig.1. Structure refinement based on a detailed structure model of p-Zn₇₅Mg₁₆Ho₉ is now under way.

References

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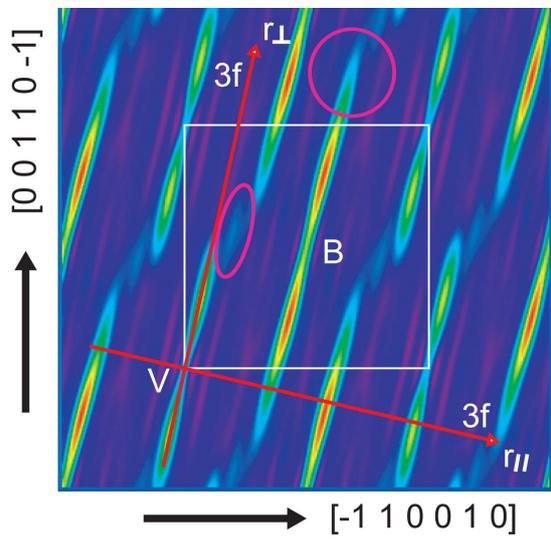


Fig. 1. 2D cut of the 6D nuclear densities containing a threefold axis in both external and internal directions.