Atomic structures of the Yb-Cd-Mg icosahedral quasicrystals and 1/1 approximants

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A discovery of binary icosahedral (i) quasicrystal (QC) $YbCd_{5.7}$ achieved a breakthrough and the description of the atomic structure is now available [1, 2]. On the other hand, the atomic structure of ternary QCs remains challenging problem because of substitutional disorder cannot be ignored in this case. To investigate the atomic structure of ternary iQC, we focused on the Yb-Cd-Mg system where iQC phases form in the wide composition range [3]. A systematic investigation has been performed on the Yb-Cd-Mg iQCs and 1/1 approximants (APs) contain very different Mg concentrations [4].

The single-grained crystals of i-Yb-Cd-Mg QCs with five different compositions have been prepared. The compositions have been analysed by ICP-AES and given by $Yb_{15.80}Cd_{77.86}Mg_{6.34}$, $Yb_{15.2}Cd_{68.4}Mg_{16.1}$, $Yb_{16.12}Cd_{58.46}Mg_{25.43}$, $Yb_{16.02}Cd_{51.33}Mg_{32.65}$ and $Yb_{15.1}Cd_{38.5}Mg_{46.4}$. In addition, we obtained single-grained crystals of 1/1 APs with three different compositions given by $Yb_{12.9}Cd_{78.4}Mg_{8.8}$, $Yb_{13.3}Cd_{70.3}Mg_{16.5}$ and $Yb_{13.3}Cd_{64.2}Mg_{22.5}$. The diffraction experiment has been carried out using in-house X-ray diffraction system (Mo target). Data reduction including integration and absorption correction has been performed using a computer package CrysAlisPRO. The atomic structures of QCs were analysed based on the 6-dimentional model of i-$YbCd_{5.7}$ [2] using 3083 common unique reflections, utilizing a computer package QUASI07 [5], and that of 1/1 APs were analysed using a refinement program SHELXL [6].

In the iQCs, it was found that there are three types of Cd/Mg occupation, namely, Cd preferential site, Mg preferential site and Cd/Mg mixed site, and the occupation probabilities of Mg atoms at the Mg preferential site show a saturation behaviour around the Mg content of 20 at.%. The results are consistent with previous report on i-$Yb_{12}Cd_{36}Mg_{52}$ QC [7]. This selective Mg occupation is identified as a cause of the non-linear increase in the icosahedral lattice constant with increasing Mg content. The 1/1 APs have a similar selective Mg occupation to that of the iQCs in terms of the shell structures of the Tsai-type rhombic triacontahedon cluster. In both iQCs and the 1/1 APs, the Mg preferential sites have a smaller number of Yb atoms among their coordination numbers. The details of resulting structures will be presented and discussed together with the observed diffuse scattering.

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