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Atomic structures of the Sc-Zn and R-Cd icosahedral quasicrystals

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We present the refinement results of atomic structures of binary icosahedral (i) ScZn7.3, GdCd7.9, DyCd7.5 and TmCd7.3 quasicrystals (QCs) [1, 2] and the study of phason modes. Bragg peak intensities data collection has been carried out on the CRISTAL beamline at the synchrotron SOLEIL, using an incoming X-ray energies equal to 25.5 keV (Sc-Zn) and 24.2 keV (R-Cd), and a CCD camera located at 8 cm from the samples. For all iQC samples a high redundancy (average 50) has been obtained resulting in 4057 (Sc-Zn) and 4871 ~ 5130 (R-Cd) unique reflections having intensity larger than 3 sigma and internal R factors around 8 %. The atomic structures of the iQCs were solved using the measured Bragg intensity data based on a six-dimensional model that is isostructural to the i-YbCd5.7 one [3] and the refinement program named qcdiff by A. Yamamoto, resulting in R factors equal to 10.9 % (Sc-Zn) and 8.9 ~ 10.9 % (R-Cd). The resulting structures are described with a quasiperiodic packing of large Tsai-type rhombic triacontahedron clusters (RTH) and double Friauf polyhedra (DFP), both resulting from a close-packing of large (Sc, R) and small (Zn, Cd) atoms. The significant difference in alloy composition between i-ScZn7.3, i-RCd~7.9 and the ideal model of i-YbCd5.7 was found to lay mainly on the DFP where one of the two large atom site (Sc, R) is replaced by a small atom (Zn, Cd) resulting in a significant distortion of the DFP. Residual disorder with relative occupancies of Sc(R)/Zn(Cd)=80/20 was also found on the icosahedral site. This illustrates that a detailed understanding of the atomic structure can now be achieved in QCs. The stabilization mechanism for these binary iQCs and the microscopic origins to explain the phason fluctuations will be discussed in this presentation.

(1) Canfield, P. C., Caudle, M. L., Ho, C. S., Kreyssig, A., Nandi, S., Kim, M. G., Lin, X., Kracher, A., Dennis, K. W., McCallum, R. W. & Goldman, A. I. (2010) Phys. Rev. B, Solution growth of a binary icosahedral quasicrystal of Sc12Zn88, 81, 020201.
(2) Goldman, A. I., Kong, T., Kreyssig, A., Jesche, A., Ramazanoglu, M., Dennis, K. W., et al. (2013). Nature Materials, A family of binary magnetic icosahedral quasicrystals based on rare earths and cadmium, 12(8), 714–718.
(3) Takakura, H., Gómez, C. P., Yamamoto, A., de Boissieu, M., & Tsai, A. P. (2006). Nature Materials, Atomic structure of the binary icosahedral Yb–Cd quasicrystal, 6(1), 58–63.

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