Structure Refinement of a Decagonal Al$_{72}$Ni$_{20}$Co$_8$ Quasicrystal by using Convergent-Beam Electron Diffraction

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The single crystal X-ray diffraction technique has so far been used, as a powerful tool, for structure analysis of quasicrystals. However, only a few quasicrystals have been analyzed because the preparation of a large single quasicrystalline grain, which is necessary for the X-ray analysis, is difficult for most of quasicrystals. In order to perform structure analysis of quasicrystals in nanometer-sized area, we have developed a structural refinement method of the quasicrystals by using convergent-beam electron diffraction (CBED). In the present study, we applied the structure analysis method to an Al$_{72}$Ni$_{20}$Co$_8$ alloy, which is known as a highly ordered decagonal quasicrystal.

An alloy of Al$_{72}$Ni$_{20}$Co$_8$ was melted in Ar atmosphere, annealed at 900 °C for 47 h and quenched in cold water. Energy filtered CBED patterns were taken at the [11110] incidence, which is one of the two-fold axes. An energy slit was set to be 10 eV to obtain zero-loss CBED patterns. The probe size of electron beam was 10 nm in diameter.

Fully dynamical CBED simulation was carried out on the basis of the Bethe method with about 250 beams including strong reflections observed in experimental CBED patterns. The structural model used in the present study consists of pentagonal (P) and Star-shaped (S) clusters with about a 0.4nm radius (FIG 1(a)), which are located at vertex positions of two different hexagon-boat-star tiling whose scales are different by τ times to each other (FIG 1(b))[1].

Structural parameters fitted in the present study were the positions of transition metal atoms, TM$^1$, TM$^2$ and Al$^1$, thickness of the specimen and scale factor. Due to the constraint of the space-group symmetry of $P10_5/mmc$, only the radial displacements of TM$^1$, TM$^2$ and Al$^1$, which are denoted as $a_1$, $a_2$ and $a_3$, respectively, are considered. These parameters were determined by minimizing a sum of residual square error $\chi^2$ calculated from intensities of experimental and simulated CBED patterns (FIG 2(a), (b)). The $\chi^2$ is calculated from six higher-order Laue zone (HOLZ) reflections as shown in FIG 2 indicated by arrows, whose intensities are sensitively changed by the displacements of the atoms. The determined parameters were $a_1 = 0.011$ nm, $a_2 = 0.030$ nm, $a_3 = 0.037$ nm, which are similar to the results of X-ray diffraction study by Takakura, $a_1' = 0.0084$ nm, $a_2' = 0.0208$ nm, $a_3' = 0.0106$ nm [2]. FIG 3 shows the experimental and simulated reflection disks used in the present fitting. The left column shows the disks simulated from the initial model without any displacement. The central column shows experimental disks. The left column shows disks simulated form the refined model. It is seen that the refined parameters well reproduce the experimental CBED disks, as are seen in the intensities indicated by arrows.

References

FIG 1. The P and S cluster model of Al$_{72}$Ni$_{20}$Co$_{8}$ decagonal quasicrystal; (a) The projection figure of Pentagonal (P) and Star-shaped (S) clusters from ten-fold axis; (b) The atom positions taken from locating the clusters at vertex positions of two different hexagon-boat-star tiling whose scales are different by $\tau$ times to each other.

FIG 2. CBED patterns taken at the Al$_{72}$Ni$_{20}$Co$_{8}$ [11110] incidence; (a) An experimental CBED pattern used the energy filter; (b) A simulation CBED pattern used P&S cluster model.

FIG 3. The experimental and simulated CBED disks. The left column shows the disks simulated from the beginning model. The central column shows experimental disks. The left column shows disks simulated form the refined model.