Symmetry Studies of ZnSc and ZnFeSc Icosahedral Quasicrystal by Convergent Beam Electron Diffraction

Shiro Miwa[1], Koh Saitoh[2], Nobuo Tanaka[2], Tsutomu Ishimasa[3], Kazue Nishimoto[4], Ryuji Tamura[5]

[1]Department of Crystalline Materials Science, Nagoya University, Nagoya, 464-8603, Japan
[2]EcoTopia Science Institute, Nagoya University, Nagoya, 462-8603, Japan
[3]Graduate school of Engineering, Hokkaido University, Sapporo 060-8628, Japan
[4]IMRAM, Tohoku University, Sendai, 980-8577, Japan.
[5]Department of Materials Science and Technology, Tokyo University of Science, Niijuku 125-8585, Japan

Quasicrystals(QCs) are matters which have non-crystallographic rotational symmetry but have a long range order. A stable binary icosahedral QC of ZnSc was found by Canfield et al [1]. The icosahedral ZnSc alloys form facetted single grains in the shape of either a pentagonal dodecahedron (PD) or a rhombic triacontahedron (RT) depending on the nominal composition. Maezawa reported that the quasicrystalline order of ZnSc QC significantly improves by introducing third elements of Mg, Ag, Fe and Pd [2]. A characteristic feature of ZnSc iQC is that the basic structural unit is Tsai-type atom cluster, which has a tetrahedral shell in its center. Icosahedral phases composed of Tsai-type atom clusters are observed in Cd-based icosahedral QCs. The Cd icosahedral QCs have a unique structural feature; that is, the lattice has a regular icosahedral symmetry but the whole atomic arrangement dose not [3]. In the present study, the symmetry of the whole structure of a ZnSc and ZnFeSc iQC is studied by the nano-beam electron diffraction (NBD) and the convergent-beam electron diffraction (CBED).

Alloys of ZnSc and ZnFeSc were prepared by the self-flux method. The nominal compositions for the PD type and RT type are $Zn_{96}Sc_4$ and $Zn_{98.5}Sc_{1.5}$, respectively. The alloys were crushed and dispersed on copper grids with holey carbon films. NBD and CBED studies were conducted using a transmission electron microscope (TEM) operated at 120 kV. Diffraction patterns were taken from specimen areas of about 100-200nm and 15nm in diameter, respectively.

Figures 1 (a), (b) and (c) show a NBD pattern of the ZnFeSc iQC and a CBED patterns taken at the fivefold axis incidence. The NBD pattern shows sharp spots which are located at the regular icosahedral positions. The lattice type of the ZnFeSc iQC was determined to be P-type because there were no systematic extinction rule in the NBD pattern. Figures 1 (b) and (c) show a CBED pattern formed by zeroth-order Laue zone (ZOLZ) reflections and a whole CBED pattern which includes higher-order Laue zone (HOLZ) reflections, respectively. The CBED pattern formed by ZOLZ reflections exhibits a tenfold rotation symmetry and two types of mirror symmetries, the resultant symmetry being expressed as 10*mm*. The pattern including HOLZ reflections exhibits a fivefold symmetry and a type of mirror symmetry, the resultant symmetry being expressed as 5*m*. Combining the symmetries of the CBED pattern taken at the threefold axis and twofold axis incidences, the space group was determined to be $Pm\bar{3}\bar{5}$.

Figures 2 (a), (b) and (c) show a NBD pattern of the ZnSc PD type iQC and a CBED patterns taken at the fivefold axis incidence. The NBD pattern shows that the lattice has a regular icosahedral symmetry. But the CBED patterns show breaking of fivefold symmetry, indicating that has no icosahedral symmetry. The symmetry breaking feature was also shown in RT type iQCs. Phason matrices, which characterize the distortion of the icosahedral lattice, were determined from relation between the displacements of the reflection and their Qperp components.

References

[1] P. C. Canfield et al., Phys. Rev. B 81, 02201(2010)
[2] R. Maezawa et al., Phil. Mag. Lett., 84,215(2004).Vol.43 (2003) L1268
[3] K. Saitoh et al., J. Cryst. Soc. Jpn., 49 34-39 (2007)

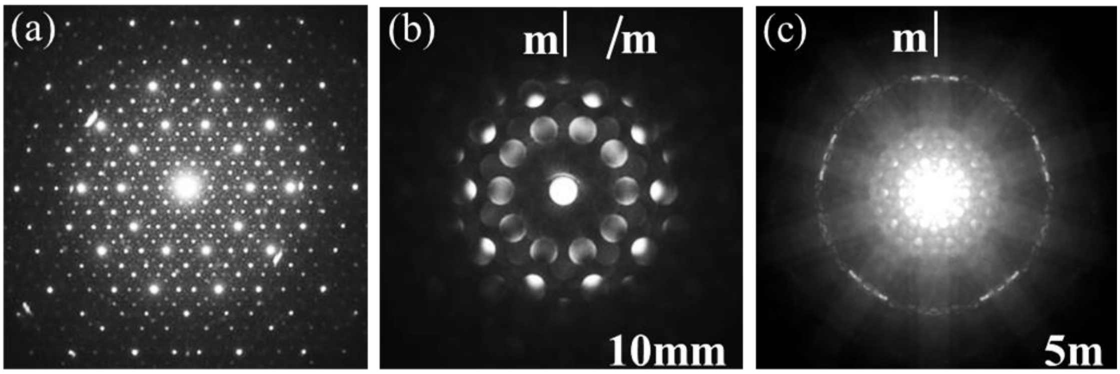

Figure 1. NBD and CBED patterns of ZnFeSc iQC at an incidence parallel to the fivefold axis. The NBD pattern (a) and the CBED pattern formed by ZOLZ reflections (b) and HOLZ reflections (c).

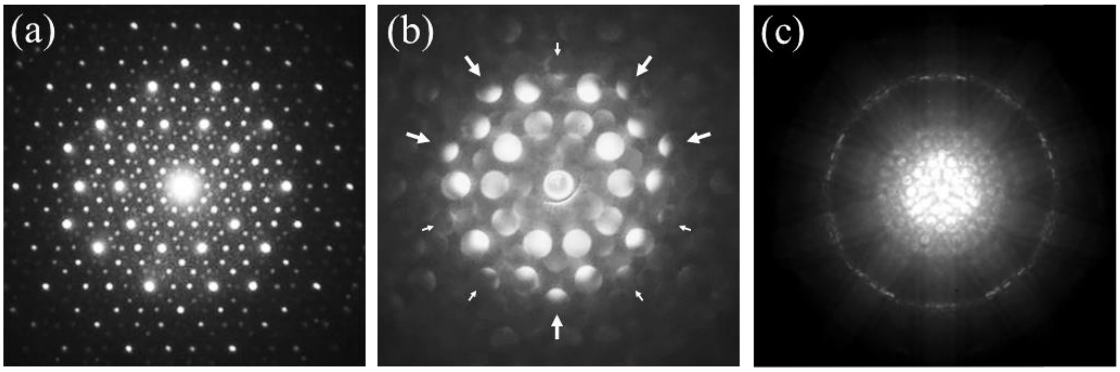

Figure 2. NBD and CBED patterns of ZnSc PD type iQC at an incidence parallel to the fivefold axis. The NBD pattern (a) and the CBED pattern formed by ZOLZ reflections (b) and HOLZ reflections (c).