Oral Contributions

[MS15-03] Structure Analysis of Approximants for Quasicrystals with 3D Electron Diffraction Tomography

Yanhang Ma[a], Peter Oleynikov[a], Nobuhisa Fujita[b], Francisco Javier García[c], Tsutomu Ishimasa[d], Osamu Teresakia,[e] .

[a]*Department of Materials and Environmental Chemistry, Stockhol University, Stockholm, Sweden.*
[b]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan.*
[c]*ICTS Centro Nacional de Microscopía Electrónica, Facultad CC. Químicas, Universidad Complutense de Madrid, Madrid E-28040, Spain*
[d]*Division of Applied Physics, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, JAPAN*
[e]*Graduated School of EEWS (WCU), Korea Advanced Institute of Science and Technology, Daejeon, Republic of Korea.*
Email: peter.oleynikov@mmk.su.se
Email: terasaki@mmk.su.se

The structural determination of quasicrystals (QCs) is still quite challenging topic.[1] The conventional techniques for crystal structure analysis usually are inapplicable for analyzing the QC cases because of the lack of translational symmetry. However, conventional techniques such as X-ray, electron and neutron diffraction will still provide much valuable information about the constituent clusters and their local packing manners.[2-4] In particular, study of analogous approximant crystals provides hints to the QCs because the crystal structure of an approximant is generally described as a periodic packing of clusters, which is also the constructing basis of the relevant quasicrystals. The understanding the structure of approximants remains a challenging and fascinating problem.

Herein, we are trying to open a new approach for a structure solution of approximants by combining the recently developed three dimensional electron diffraction tomography (3D-EDT) [5] and scanning transmission electron microscopy (STEM) images (both BF and HAADF). Similar to single X-ray diffraction (XRD) technique, we can obtain 3D ED data set from a nanocrystal by 3D-EDT through combining crystal and beam tilt to sweep 3D reciprocal space in a designed manner. We need to improve further the method in order to collect data more precisely in terms of reflection intensity and its position in reciprocal space. The structure can be solved using direct method or charge flipping on basis of electron diffractions in 3D reciprocal space. STEM images gave the information about the positions of heavy atoms and local defects in the structure, which can be used to relate the structure between approximant and QCs. Zn-Sc approximant ($Zn_{85.5}Sc_{14.5}$) and Al-based F-type ($Al_{69.1}Pd_{22.8}Fe_{6.0}Cr_{2.1}$) cubic approximants were used to verify the feasibility and power of 3D-EDT method on solving approximants for QCs.

Figure 1a shows one slice cut from reconstructed 3D EDT data along [100] direction. The space group was determined as *Im*-3 with $a = 14$ Å. 561 unique reflections have been extracted for the Zn-Sc approximant[6] to solve its structure. The electrostatic potential map (Figure 1b) obtained using direct method shows the projection of atoms along [100] direction, which coincides with the structural model in the databse[7]. Over 30,000 reflections were collected for the F-type approximant due to its large unit cell parameter ($a = 40.5$ Å). And the Laue group was determined to be *m*-3 with reflection absence conditions: *0kl: k*=2n; 00*l*: *l*=2n. This will leads to the non-centrosymmetric space group *Pa*-3 uniquely. The rough structural model has been solved based on the extracted electron diffraction. Many atoms can be found in the model. The detailed structural information will be discussed in the conference.

Figure 1. a) Slice cut from 3D EDT data along [100], b) electrostatic potential map along [100] solved by direct method based on 3D EDT data and c) structural model of Zn-Sc approximant from the ICSD database[7].

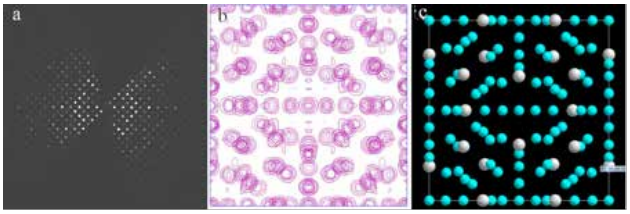


Figure 2. a) ED patterns from 3D EDT along a) [111], b) [100] , c) [010] and d) [001] zone axis.

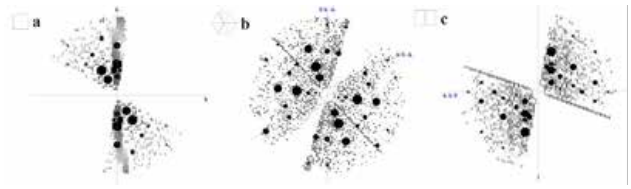
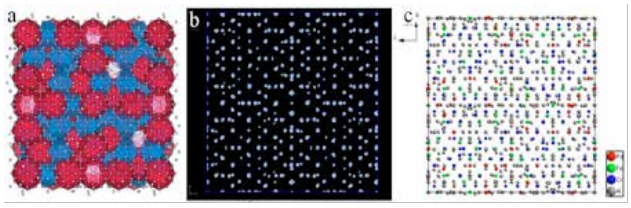


Figure 3. a) Structure model solved by Fujita et al using single X-ray, b) electrostatic potential map and c) structure model solved by 3D EDT data of the Al-based F-type cubic approximants.



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