

## DIRECT 3D ATOMIC ARRANGEMENT ANALYSIS BY ATOMIC RESOLUTION HOLOGRAPHY AND STEREOGRAPHY

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3D local atomic structure around specific active-site atom, such as a dopant in Si crystal, plays crucial role in a functional materials. The 3D atomic structure analysis around this kind of local specific atom, however, has not been possible by a standard structure analysis method because this kind of active site has no translational symmetry.

The angular distribution of core-level photoelectrons from the atom in x-ray photoelectron spectroscopy (XPS) can reveal 3D atomic structure around specific atoms, and is called photoelectron holography. Recently its accuracy improved dramatically by the development of new analysis code [1]. A new technique of direct 3D atomic structure analysis method "stereography of atomic arrangement" has also been developed [2]. Because the accuracy of the atomic structure analysis has become high enough for practical applications, we started a project of "3D active-site science" [3]. The target materials in this project ranges from inorganic to bio-materials.

Figure 1 shows an example of photoelectron holography from superconductor graphite intercalation compound  $\text{Ca}_{0.11}\text{K}_{0.89}\text{C}_{7.1}$  [4]. We can see clear carbon honeycomb structure and K atoms arranging 2x2 structure. An example of stereography [5] is shown in Fig. 2, which is a direct 3D image of atomic arrangement viewed from an In atom in InP crystal toward [111] direction. The atom A looks closest to you if you see the left and right pictures by your left and right eyes, respectively. These techniques realized an emergence of a new local structure science. [1] A. Leng, H. Streckel, M. Stratmann, Corros. Sci. 41 (1998) 547.

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[2] H. Daimon: Phys. Rev. Lett. 86, 2034 (2001).

[3] URL: <http://www.en.3d-activesite.jp/>

[4] F. Matsui et al.: Scientific Reports 36258 (2016).

[5] T. Matsumoto, et al.: e-J. Surf.Sci. Nanotech. 7, 181 (2009).

Figure 1

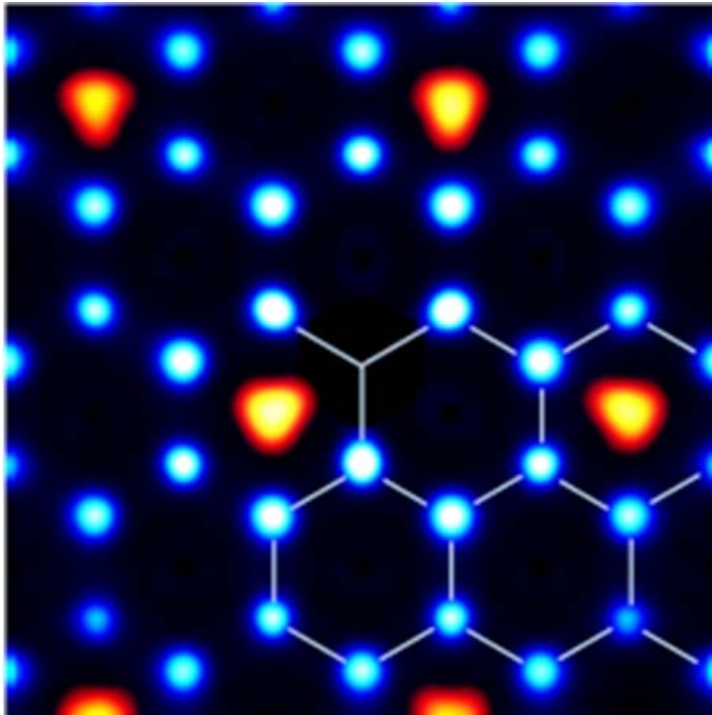


Figure 2

