Photoelectron Holography: Maximum Entropy Reconstruction Scheme

Holography utilizing the wave nature of electrons was originally proposed by Gabor [1] for the electron microscope. In his technique, a point source, i.e., a highly focused electron beam is utilized, and the size of the point source correlates with spatial resolution. Sz_ke pointed out that atomic resolution holography can be realized by utilizing a wave emitted from an atom [2] (characteristic X-ray, photoelectron or Auger electron), which is an atomic scale point source. A schematic view of photoelectron holography is shown in Fig. 1. The emitted wave is partially scattered by the potentials of surrounding atoms, and an interference pattern between the unperturbed and scattered waves is observed in the angular distribution. The pattern is interpreted as a hologram recording the three-dimensional atomic arrangement. It has been expected that the local atomic structure around the target atomic site can be directly obtained from the hologram, since an emitter atom is selective by choosing the photoelectron energy characteristic to the element and chemical state. Barton proposed a numerical algorithm on the basis of the Fourier transform [3] to reconstruct a three-dimensional atomic arrangement from an electron hologram. However, the image from an actual single-energy hologram was unclear, due to the forward scattering effect, i.e., strong intensity of forward focusing peak and the frequency shift around the forward scattering region prevent the simple Fourier analysis. To avoid the effect of forward focusing peaks, many techniques have been developed such as the multi-energy method [4], and differential hologram [5] among others. However, the reconstruction from a single-energy hologram has been quite difficult.

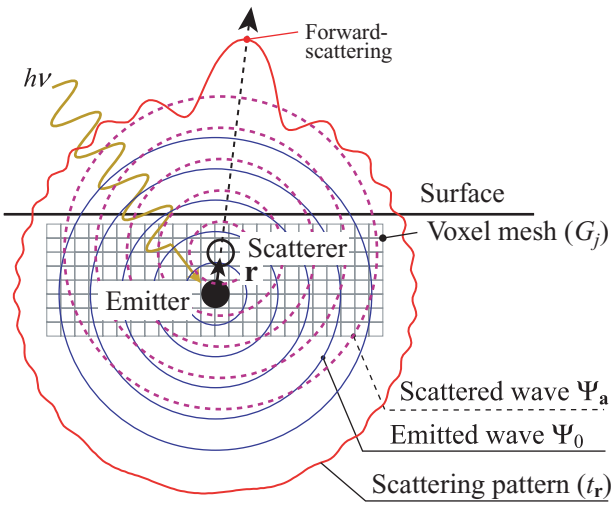

Fig. 1. Schematic view of photoelectron holography.

We have proposed a new algorithm using the maximum entropy method to single-energy photoelectron holography. It is composed of the scattering pattern matrix and the maximum entropy method [6,7]. The idea is quite simple. We have defined a new mathematical expression of the hologram as

$$\chi(\vec{k}_i) \equiv I(\vec{k}_i) - |\Psi_0(\vec{k}_i)|^2,$$
$$\cong \sum_j t_{\vec{a}_j}(\vec{k}_i) \cdot G_j$$

where $\chi(\vec{k})$ is the hologram function, $I(\vec{k}_i)$ is the measured intensity, $\Psi_0(\vec{k}_i)$ and is the photoelectron wavefunction from the emitter (reference wave). $t_{\vec{a}_j}$ is a scattering pattern caused by a scatterer atom located on $\vec{a}_j$. Here, the real space voxel is defined as **G**, and its element located on $\vec{a}_j$ is described as G_j. When the elements G_j located on scatterer positions are set to $1/|a_j|$ and the others are set to 0, this formula gives the hologram pattern. This equation can be interpreted as a simple linear simultaneous equation.

Therefore, to obtain the atomic arrangement from the hologram, it is necessary to solve this linear simultaneous equation. However, it is difficult to solve it using commonly used gradient methods, because the amount of the unknown elements G_j is larger than that of the linear equations. We have found that the maximum entropy method of iterative scaling algorithm is effective for solving this equation.

To demonstrate the effectiveness of the algorithm, we measured a photoelectron hologram of Si(001) using a two-dimensional display type analyzer at beamline **BL25SU** [8]. The unique analyzer can measure an angular distribution of ±60° at once. Therefore, it can measure the photoelectron hologram within 1 sec ~ several minutes, which is quite fast. The kinetic energy of photoelectron from Si 2*p* core level was set to 800 eV. The obtained hologram is

shown in Fig. 2. Although symmetrical operation has not been applied to it, four-fold symmetry is clearly seen in the figure.

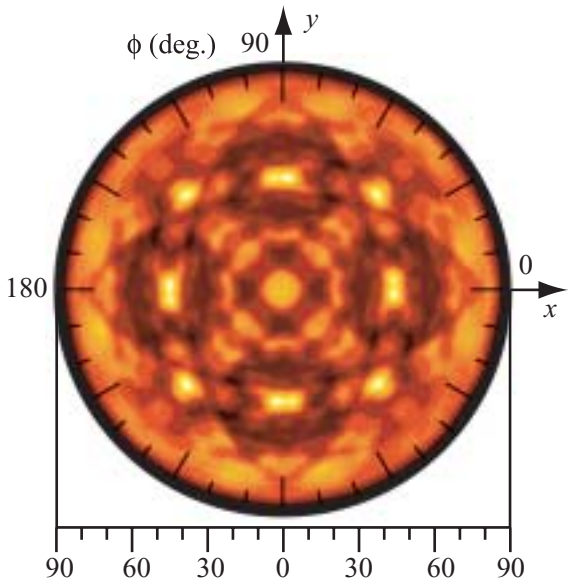

Fig. 2. Photoelectron hologram of Si(001). The initial state is Si 2*p* and the kinetic energy is 800 eV.

We applied the simple Barton algorithm (Fourier transform) and our algorithm, which are shown in Fig. 3 and Fig. 4, respectively. The simple Barton algorithm cannot reconstruct atomic image. On the other hand, the image using our algorithm is quite clear. This indicates the effectiveness of the new algorithm.

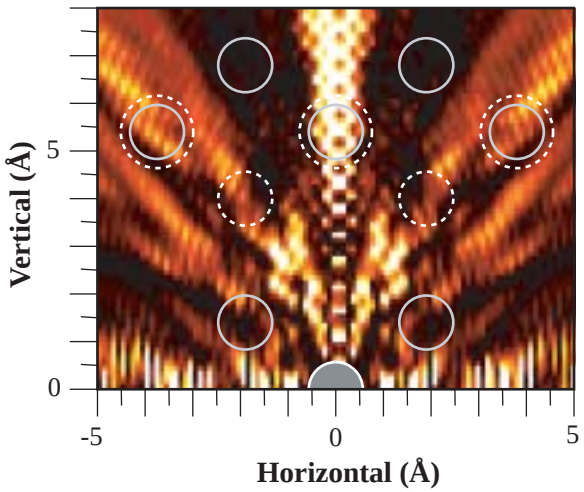

Fig. 3. Real space image of (110) plane reconstructed by simple Barton algorithm.

The combination of this algorithm and 2D-PES enables us to measure local structure around a target atomic site in real-time. This algorithm is expected to become a powerful tool for measuring atomic arrangement around a target atom.

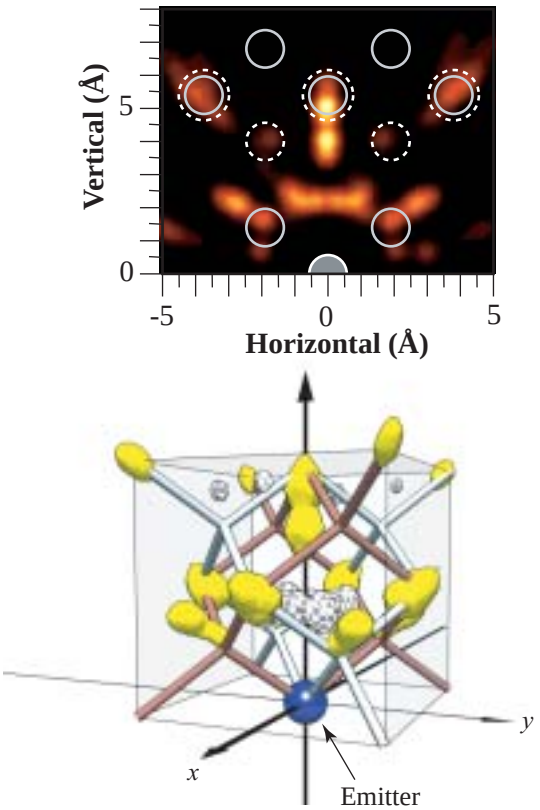

Fig. 4. Real space image of (110) plane and three-dimensional image reconstructed by new algorithm.

T. Matsushita

SPring-8 / JASRI

E-mail: matsusita@spring8.or.jp

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