3-D Imaging around a Dopant in Si Crystal by X-ray Fluorescence Holography

The doping technique in crystalline Si has played an important role in the fabrication of advanced semiconductor devices, which requires state-of-the-art tailoring of a band gap. In order to understand the nature of doping-induced electronic states, it is essential to study the local structures around impurities in a doped semiconductor. The X-ray absorption fine structure (XAFS) method is commonly used for studying the local structure of particular elements. X-ray fluorescence holography (XFH) [1,2] is a promising new technique for imaging 3-D atomic arrangements around atoms emitting fluorescence photons. This technique is also applicable to investigate the environment around a dopant [3].

The "normal" and "inverse" modes exist in the XFH method. In the normal XFH method, fluorescent X-rays from atoms in a sample with and without being scattered by surrounding atoms serve as the object and reference waves, respectively. A holographic pattern is recorded by scanning a detector around the sample. In the inverse mode, fluorescence is used to detect an interference field originating from incident and scattered X-rays (Fig. 1). The holographic pattern is obtained by detecting the fluorescence while the sample's orientation is varied relative to the incident beam. The inverse mode was preferably used in the XFH experiment at this synchrotron radiation facility because the holograms can be recorded at any incident energy above the absorption edge of an emitter.

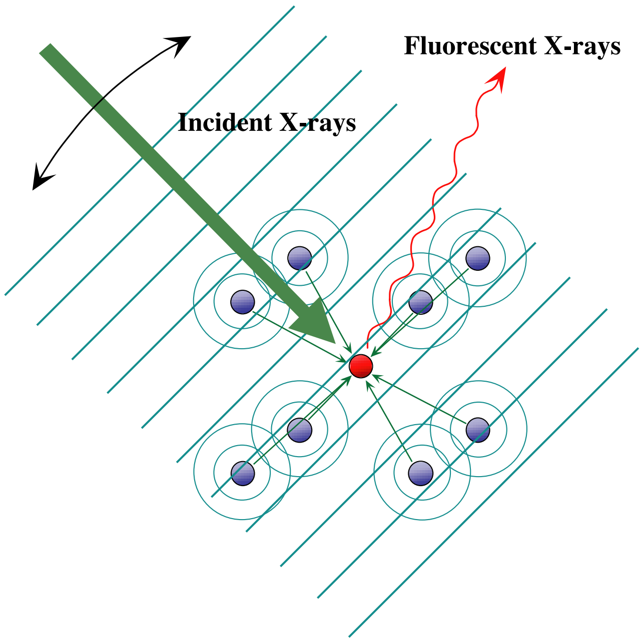
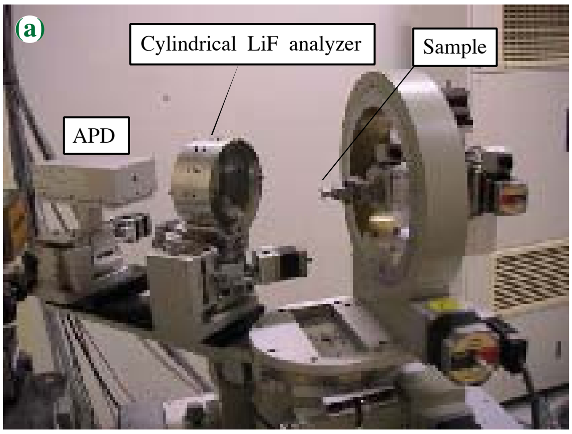


Fig. 1. The XFH principle for the inverse mode.

XFH patterns were measured at beamline **BL47XU**. An $Si_{0.999}Ge_{0.001}$ sample grown by the Czochralski method was used as the sample [4], and its dimensions were 5 × 5 × 2 mm^3. Incident energies were 14.5 - 17.0 keV with 0.25 keV steps. Figure 2 shows an experimental setup for recording inverse XFH holograms. The Ge Kα (9.87 keV) X-ray fluorescence via a cylindrical LiF crystal was detected by an avalanche photodiode. The X-ray fluorescence count rate was about 200,000 cps. The fluorescence intensities were measured as a function of azimuthal angle ϕ and polar angle θ_1 within the ranges of 0° ≤ ϕ ≤ 360° and 0° ≤ θ_1 ≤ 76°. The X-ray exit angle of θ_2 was fixed at 45°. In this experiment, we recorded 11 holograms at different energies.



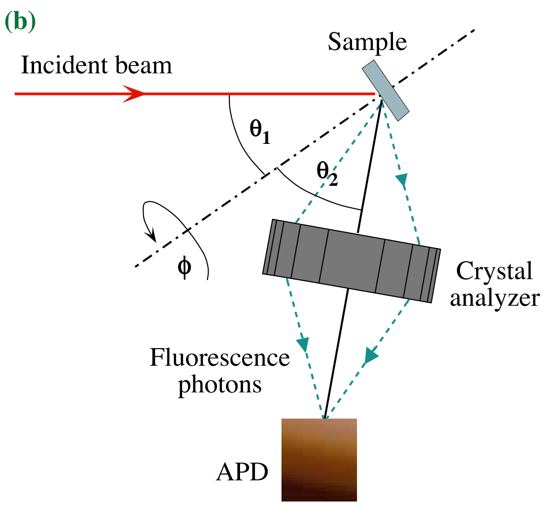


*Fig. 2. Photograph **(a)** and schematic diagram **(b)** of the experimental setup installed at SPring-8 for the structural analysis of condensed systems by XFH.*

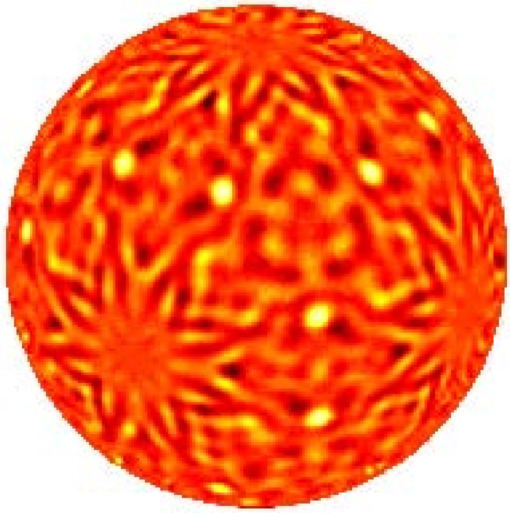


Fig. 3. Ge X-ray fluorescence hologram of $Si_{0.999}Ge_{0.001}$ recorded at 14.5 keV. The displayed pattern was obtained by symmetrization and low-pass filtering.

To handle the data, we incorporated extension of the hologram to the full sphere by using measured symmetries and low-pass filtering. Figure 3 shows the resulting hologram pattern at 14.5 keV. Multiple energy reconstruction by the Helmholtz-Kirchhoff transformation modified according to Barton was applied to these hologram data. The real space image was depicted in Fig. 4. The atomic images were extremely fine, and artifacts, which were obvious in the reconstruction by the single energy XFH, were sufficiently suppressed. The atoms up to the seventh coordination shell were recognized, though we have only displayed the atoms up to the fourth coordination shell in the Fig. 4 because of the complication of the figure. The arrangement of the atoms in the reconstruction remarkably shows a superposition of two associated environments of a diamond structure, revealing that Ge atoms lie in two distinct crystallographic sites. Thus, we found that Ge atoms are substituted for Si sites. Taking into account the Ge concentration, most of the atomic images were regarded as being of Si. Originally, XFH was weak at imaging light atoms such as Si and O. The present result revealed that our experimental and data processing techniques significantly improved the results [5].

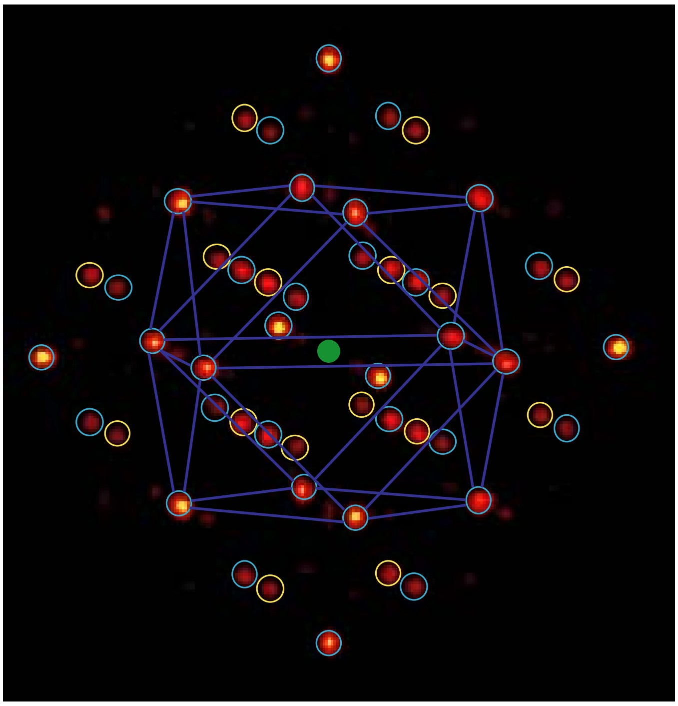


Fig. 4. 3-D image of the atomic environment around Ge in $Si_{0.999}Ge_{0.001}$.

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