CAPACITANCE XAFS: SITE-SELECTIVE OBSERVATION OF CARRIER TRAPS IN SEMICONDUCTORS

Since the XAFS spectrum is obtained by measuring the X-ray absorption with an inner-shell excitation of a specific atom, the information related to the atom and its chemical environment can be obtained even though the atom is buried in a compound. However, if the atom has various local structures dependent on its chemical environment, the XAFS spectrum provides the average information of these local structures. This causes ambiguity of the XAFS analysis in relating the microscopic local structure to macroscopic material properties. Accordingly, there is a need for a site-selective XAFS, in which only the specific minor structure in the bulk structure can be detected.

We propose the "capacitance XAFS" by measuring the photon-energy dependence of the capacitance of the Schottky barrier diode as the site-selective XAFS for the local structure analysis of the low density carrier traps in semiconductors [1]. The concept of capacitance XAFS is shown in Figure 1. The DX center of AlGaAs:Se, which is a typical deep-level electron trap, is used as an example in this figure. In AlGaAs:Se, group-VI Se substitutes for the group-V site as the electron donor and is surrounded by group-III atoms. Under X-ray irradiation of this Schottky barrier diode, a core hole is formed in the Ga K-shell by X-ray absorption. If Ga in the DX center is excited, it is expected that the localized electron drops into the core hole, as shown in Figure 1(a). Since the capacitance is proportional to the square root of the number of this electron relaxation in the carrier trap, the capacitance increases. In contrast, when the excited Ga is in the bulk AlGaAs instead of the DX center, it is relaxed by the capturing of the photoelectron, as indicated in Figure 1(b). In this case, the capacitance is not changed, while the conventional XAFS by fluorescence detection predominantly reflects this absorption. Therefore, the photon-energy dependence of the capacitance is considered to correspond to the XAFS spectrum of only Ga in the DX center.

The capacitance XAFS analysis is applied to the observation of the DX center in $Al_{0.33}Ga_{0.67}As$:Se. The sample is grown by molecular beam epitaxy on a (100)-oriented n-type GaAs substrate. The Se concentration is $5 \times 10^{17}/cm^3$. For the metal electrode of the Schottky diode, an Al dot ~0.5 mm in diameter and a thickness of ~100 nm is deposited by an evaporator. The hard X-rays can pass through this Al electrode. Experiments using synchrotron radiation are performed at the beamline **BL10XU**, a high brilliance XAFS station. The capacitance is measured by a capacitance meter with a 1 MHz oscillator.

As shown in Figure 2, a clear capacitance jump at the Ga K-edge and a XAFS oscillation are observed using this method (solid line). The conventional XAFS spectrum obtained using a solid state detector (SSD) is also shown in this figure (dashed line). An

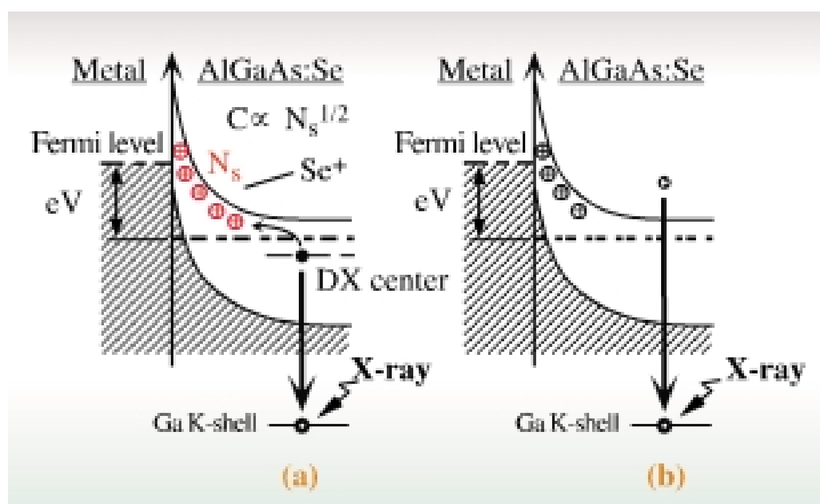

*Fig.1: Concept of the capacitance XAFS. X-ray absorption by carrier-trapping atoms **(a)** rather than bulk atoms **(b)** induces capacitance variation.*

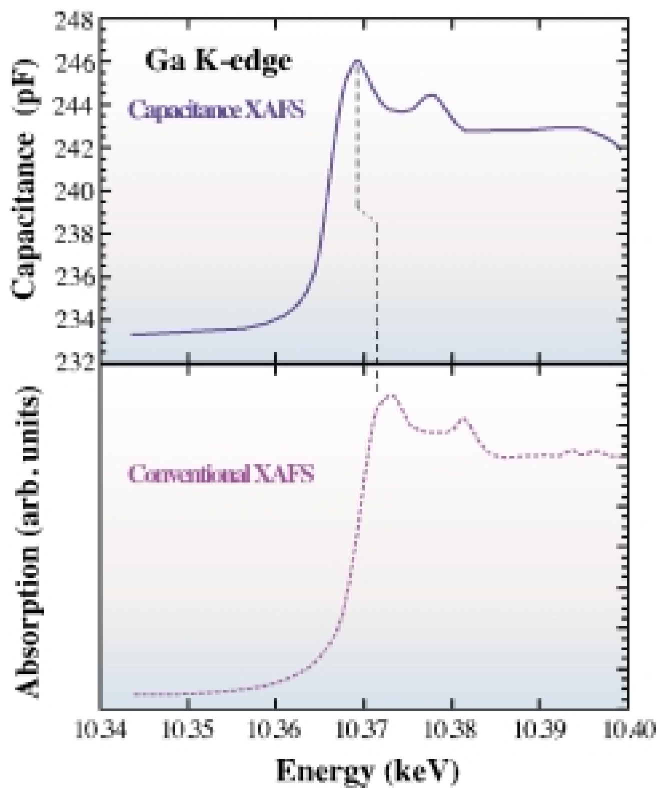

Fig.2: Photon-energy dependence of the capacitance of AlGaAs:Se at around Ga K-edge (solid line). The conventional XAFS spectrum obtained by using the SSD is also shown by dashed line.

energy shift of the absorption edge toward the low-energy side is observed in the capacitance XAFS, suggesting that only the Ga (<5x10^{17}/cm^3) neighboring Se, which constructs the DX center mixed in the bulk Ga (~1x10^{22}/cm^3), is selectively observed by the capacitance XAFS. The energy shift is considered to indicate the change in atomic coordination of Ga in the DX center. The capacitance XAFS spectrum provides direct evidence for the large lattice relaxation (LLR) model [2], in which Ga as the nearest neighbor of Se is displaced from the lattice site, instead of the donor itself, with the Ga-Se bond breaking.

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References

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