

## Capacitance XAFS method: X-ray absorption spectroscopy of low-dimensional structures

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For local structure analyses of low-dimensional structures in semiconductors, such as defects, interfaces and surfaces, a new site-selective x-ray absorption fine structure (XAFS) measurement, 'capacitance XAFS method', is presented. This method measures the x-ray photon energy dependence of the capacitance involved in diode structures. Since the capacitance is changed by an x-ray induced photoemission of localized electrons in the low dimensional structures, a site-selective analysis can be made. Although macroscopic x-ray absorption can be measured by conventional XAFS analyses, low-dimensional x-ray absorption coefficients are observed by the capacitance XAFS measurements.

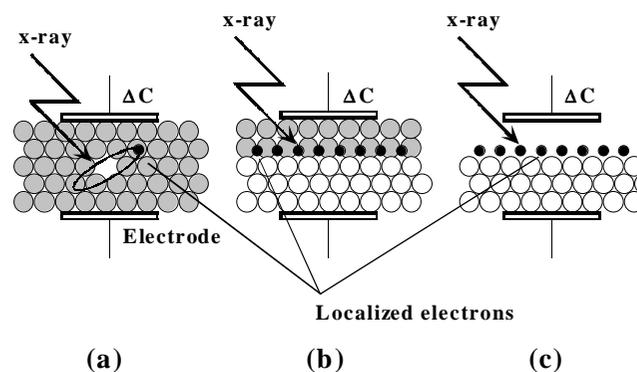
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### 1. Introduction

X-ray absorption fine structure (XAFS) measurement (Lytle *et al.*, 1975) is an important experimental technique for local structure analyses using synchrotron radiation (SR). Since the XAFS appears around the absorption-edge energy intrinsic to individual atoms, the local structure and electronic state of a specific atom can be selectively obtained even though the atom is buried in a compound. In XAFS analysis, microscopic information, such as bond lengths and the coordination number, is derived from the macroscopic absorption properties, and thus structural homogeneity of the sample is necessary. When the sample is heterogeneous with various local structures, the XAFS spectrum provides only the averaged information of these local structures. Heterogeneous systems are not only common but also of interest in current material science. For instance, the defects in a crystal, heterointerfaces and surfaces are typical example that many researchers have tried to understand their local structures. In this report, a new site-selective XAFS measurement, 'capacitance XAFS method' (Ishii *et al.*, 1999), is presented. The capacitance XAFS method provides microscopic absorption property of only the low dimensional structure in the heterogeneous systems.

### 2. Capacitance XAFS method

As shown in Fig. 1, excessive electrons are frequently localized at low-dimensional structures such as (a) defects, (b) interfaces and (c) surfaces because a deep potential energy caused by the structural modifications traps free electrons in the solids. These low-dimensional structures with localized electrons determine the electrical conductivity, optical property, and chemical reactivity of the material. The property of a trap center being different from the bulk is utilized for site-selective observation in the capacitance XAFS method. Fig. 1 shows that a couple of electrodes holding the sample makes a capacitor, which is sensitive to the amount of localized electrons in the sample. When the x-ray is irradiated into the capacitor and is absorbed at the low-dimensional structures, a photoemission of the localized electrons from the trap center is induced. The de-localized electrons are swept out from the sample,



**Figure 1**  
Low-dimensional structures observable by capacitance XAFS method: (a) defect, (b) interface, and (c) surface with localized electrons.

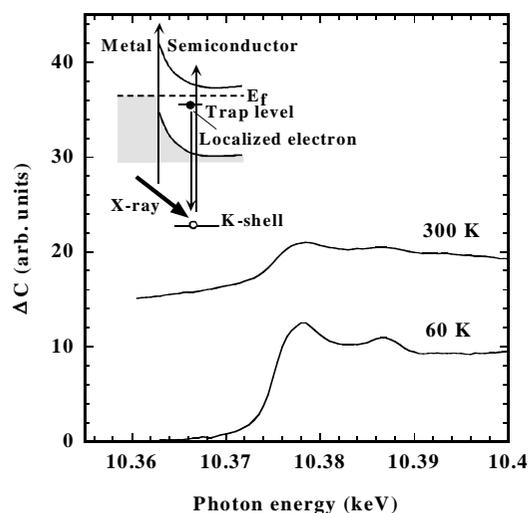
resulting in a capacitance change of  $\Delta C$ . The  $\Delta C$  can be separately detected from a resistance variation,  $\Delta R$ , caused by an x-ray induced photocurrent in the bulk. Note that the photocurrent is observed in conventional XAFS measurements. Since the  $\Delta C$  is determined by the amount of the x-ray absorption of only the low-dimensional structures, the site-selective XAFS spectra may be obtained by the photon energy dependence of the capacitance.

### 3. Experiment

Experiments were performed at SPring-8 BL10XU, the High Brilliance XAFS station (Oyanagi *et al.*, 2000). An in-vacuum-type undulator was used as a light source in this beamline. A Si (111) double crystal with a water coolant monochromatized the intense x-ray from the undulator. The sample was Se-doped  $\text{Al}_{0.33}\text{Ga}_{0.67}\text{As}$  (AlGaAs:Se) with the defect caused by a chemical property of the Se impurity (Mizuta & Kitano, 1988). A thin Al electrode of 100 nm thickness was evaporated on the sample, and the x-ray was irradiated through this electrode. A capacitance meter with a 1 MHz oscillator was connected to the electrode. The substrate temperature during XAFS measurements was controlled by a He cryostat with a 5 W heater.

### 4. Results and discussion

As shown in the inset of Fig. 2, the difference in the work function between the Al electrode and the AlGaAs:Se semiconductor forms a band bending, resulting in a depletion layer without charge in the semiconductor. This is the well-known structure called the Schottky barrier diode. The sandwich structure of the conductive metal, the insulative depletion layer, and the conductive semiconductor make a capacitor equivalent to the conceptual diagram shown in Fig. 1 (a). Therefore, the capacitance of this structure is sensitive to the localized electrons at the defect in the semiconductor. Fig. 2 shows the capacitance XAFS spectra at 300K and 60K. A clear edge-jump and XAFS oscillation are observed at low temperature. The edge-jump corresponds to the Ga K-edge (10.375 keV). This result indicates that the XAFS spectrum is obtained by the capacitance change under the SR. In contrast to the low-temperature measurement, the edge-jump becomes ambiguous at 300K. It is well known that the conventional XAFS measurement at low temperature has a clearer oscillation signal than that observed at room temperature, owing to the suppression of a thermal vibration

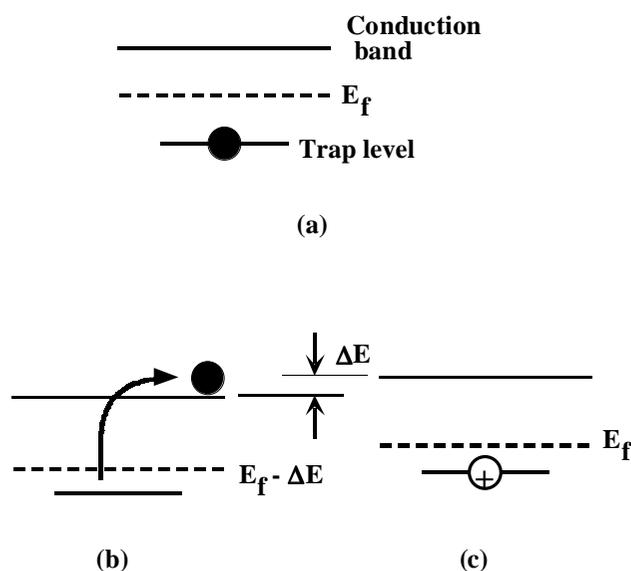

**Figure 2**

Capacitance XAFS spectra at substrate temperatures of 300 K and 60 K. A Schottky barrier diode (inset) is fabricated to measure the sample's capacitance.

of the sample atoms (Teo & Lee, 1979; McKale *et al.*, 1988). However, since the photocurrent and temperature insensitive x-ray fluorescence are used to estimate the amount of x-ray absorption, the influence of the substrate temperature on the edge-jump is negligible in conventional XAFS measurements. The temperature dependence observed in Fig. 2 provides evidence that the photoemission of the localized electrons is related to the capacitance XAFS measurement. Since the valence state has an energy level of  $\sim eV$ , the photoemission process of the localized electrons is sensitive to the temperature (Ishii *et al.*, 2000).

Fig. 3 shows a possible photoemission dynamics in this system. Only the energy diagram around the Fermi level,  $E_f$ , is illustrated in this figure. Fig. 3 (a) indicates a steady state before the x-ray irradiation. The localized electrons occupy the trap level in the band gap of the semiconductor. When the x-ray is absorbed at the defect atom, (b) excitation of the localized electrons into a conduction band is expected. The de-localized electrons are swept out from the depletion layer so that the positively charged trap center pushes down the  $E_f$  to  $E_f - \Delta E$ . The Fermi level of the semiconductor should be equal to that of the metal electrode. Consequently, (c) the energy level of the conduction band is increased by  $\Delta E$ . This level modification reduces the thickness of the depletion layer, resulting in the capacitance increment of  $\Delta C$  by the x-ray absorption. Since there is no trap level in the bulk, the photoemission shown in Fig. 3 is not induced.

The point and line defects have zero- (0-D) and one-dimensional (1-D) structures, respectively, indicating that 0-D and 1-D x-ray absorption coefficients are obtained by the capacitance XAFS measurements. Two-dimensional (2-D) x-ray absorption is similarly obtained from the capacitance XAFS spectra of an interface atom with localized electrons at dangling bonds as illustrated in Fig. 1 (b). Although macroscopic 3-D x-ray absorption can be measured by conventional XAFS analyses of the bulk atom, 0-2-D x-ray absorption coefficients in a 3-D sample are defined by the site-selectivity of capacitance XAFS measurements. Moreover, capacitance XAFS measurements using a scanning capacitance microscope (SCaM-XAFS), in which a microprobe is used for the


**Figure 3**

Schematic band diagram of photoemission in capacitance XAFS measurement. (a) Steady state before the x-ray irradiation, (b) excitation of the localized electrons into a conduction band, and (c) reduction of the depletion layer thickness by the excitation (b).

capacitance detection, and the air gap capacitor indicated in Fig. 1 (c) are expected to evaluate the 0-2-D x-ray absorption on a 2-D sample surface. These low-dimensional x-ray absorption coefficients make it possible to analyze the heterogeneous systems by the XAFS method.

## 5. Summary

Capacitance measurement is utilized for detection of the x-ray induced photoemission of localized electrons. By extending this technique, a new site-selective x-ray absorption fine structure (XAFS) technique, called the capacitance XAFS method, has been developed. The photon energy dependence of the capacitance is expected to be the XAFS spectra of only the low-dimensional structures with the localized electrons. The capacitance XAFS spectrum of Se-doped AlGaAs with a defect was successfully obtained. In this system, the photoemission of localized electrons forms a positively charged trap center, which modifies the width of a semiconductor's depletion layer, resulting in a capacitance change corresponding to the x-ray absorption. The site-selectivity involved in the capacitance XAFS method defines low-dimensional x-ray absorption coefficients in heterogeneous systems.

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