

## PHOTOEMISSION PROCESS OF A LOCALIZED ELECTRON IN CARRIER TRAP AND ITS APPLICATION TO SITE-SELECTIVE X-RAY ABSORPTION FINE STRUCTURE MEASUREMENT

X-ray absorption fine structure (XAFS) measurement is an important experimental technique, which uses synchrotron radiation (SR) for local structure analyses. In XAFS analysis, microscopic information, such as bond lengths and the coordination number, is derived from the *macroscopic* absorption property, and thus structural homogeneity of the sample is necessary. When the sample is heterogeneous with various local structures, the XAFS spectrum provides only the average information of these local structures. A meaningful analysis using this average information is impossible, except in the rare case in which the spectrum can be deconvoluted into a few spectra of some well-known structures. A heterogeneous system is not only common but also is of interest in current material science. For instance, the defects in a single crystal and heterointerfaces fabricated by epitaxial growth have singular structures in the crystal. The assumption of sample homogeneity restricts the applicability of XAFS measurement.

Recently, we proposed a new XAFS method, capacitance XAFS measurement [1]. In this method, since the amount of X-ray absorption is evaluated by a capacitance change due to Xray induced photoemission of a localized electron, a site-selective XAFS analysis of the specific atoms with the localized electron may be achieved. It is well known that the defects and dangling bonds at the heterointerface in semiconductors localize electrons owing to their characteristics as trap centers, suggesting that the *microscopic* absorption property of these singular atoms can be selectively analyzed by capacitance XAFS measurement. In this research, the X-ray induced photoemission property of the localized electron and the siteselectivity of capacitance XAFS measurement based on this process are discussed.

The detailed concept and experimental apparatus of capacitance XAFS method were described in previous papers [1,2]. In our experiments performed at the High Brilliance XAFS beamline **BL10XU**, the capacitance involved in the Schottky diode of a compound semiconductor, Se-doped AlGaAs, was measured under SR irradiation. It is well know that a deep level of the electron trap, the DX center, is formed in this sample due to the intrinsic property of the donor impurity in zinc-blende semiconductors.

Figure 1 shows the capacitance XAFS spectra at the Ga K-edge (10.375 keV). The sample







temperature was varied from 60 K to 300 K. As shown in this figure, the edge jump decreases with increasing substrate temperature, and finally, it almost disappears at room temperature. This tendency is in contrast to that of the conventional XAFS method. In conventional fluorescence XAFS method, since the X-ray penetration depth and escape depth of the fluorescence, which are independent of the sample temperature, determine the number of detectable atoms, no temperature dependence of the edge-jump is observed. On the other hand, the valence electronic states are easily modified by thermal energy of the order of ~ meV. The temperature dependence of edge-jump in Fig. 1 provides evidence that the valence electron is related to the signal-detection process in capacitance XAFS measurement. In fact, the activation energy of the photoemission process of trapped electron is estimated to be 7.33 meV from a fitted result of the temperature dependence based on the Arrhenius' equation as shown in Fig. 2.

Moreover, a capacitance-voltage (C-V) analysis which provides the carrier concentration in the semiconductor, indicates that the activation energy of the extra donor generation process under SR is evaluated to be 7.68 meV [2]. Almost the same activation energies for the photoemission in capacitance XAFS measurement (7.33 meV) and this extra donor generation indicate that the signal amplitude of capacitance XAFS measurement is determined by the X-ray induced photoemission of the localized electron to conduction band in the semiconductor. This is consistent with the concept of capacitance XAFS method.

Figure 3 shows a possible photoemission dynamics based on these finding. Only the energy diagram around the Fermi level,  $E_f$ , is illustrated in this figure. The 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



*Fig. 2. Arrhenius' plot estimation of thermal activation energy of the photoemission process in the capacitance XAFS method.* 





electrons into a conduction band is expected (Fig.3 (b)). 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 used for the capacitance formation. Consequently, (c) the energy level of the conduction band is increased by  $\Delta E$  (Fig.3 (c)). The level modification reduces the thickness of the

depletion layer without the localized electron, resulting in the capacitance increment by the Xray absorption. This dynamics indicates the *microscopic* X-ray absorption at the defect, not the *macroscopic* absorption at bulk, is selectively obtained by capacitance XAFS method. The details of structural analysis using XAFS method are described in SPring-8 Research Frontiers 1997/1998 [3].



Fig. 3. Possible photoemission dynamics in capacitance XAFS measurement.

Masashi Ishii

SPring-8 / JASRI

E-mail: ishiim@spring8.or.jp

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