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Structural Analysis of GaInN Single Quantum Well using X-ray Absorption Fine Structure

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Although $Ga_{1-x}In_xN$ quantum wells have been used for the emitting layer of a GaN-based laser diode, which is a key device in high-density optical storage systems, there is a serious problem in that phase separation is occasionally observed in $Ga_{1-x}In_xN$ alloy with a high indium content ($x>0.20$). This separation can be ascribed to the large lattice-constant difference between GaN and InN, but the details are not known. We have already analyzed the local structures around In atoms of $Ga_{1-x}In_xN$ layer [1] and $Ga_{1-x}In_xN$ /GaN multi-quantum wells [2] using the fluorescence-detecting x-ray absorption fine structure (XAFS) method. Here we investigated $Ga_{1-x}In_xN$/GaN single quantum wells, which is useful for the above discussion although it is difficult to obtain the XAFS signal because of the thin layer.

As a sample, a 2μm-thick GaN layer was grown on a sapphire substrate using metal-organic chemical vapor deposition (MOCVD), followed by a single quantum well of $Ga_{0.92}In_{0.08}N$ (4.5nm thick). Fluorescence-detecting XAFS experiments were performed at BL01B1 of SPring-8 using synchrotron radiation from the 8 GeV storage ring. The x-ray was monochromated by two Si (111) crystals and irradiated on the sample. Fluorescence x-ray was obtained from the sample and detected by a Ge solid-state multi-detector with 19 elements.

Figure 1 shows the In K-edge fluorescence-yield spectrum for a $Ga_{0.92}In_{0.08}N$/GaN single quantum well measured at 300K. The intensity of fluorescence x-ray was corrected in order to reflect the solid-state detector's inability to accurately detect high-intensity x-ray. The absorption K-edge of In atoms was observed near the excited photon energy of 27.94 keV. A clear fine structure was also observed at an energy above the In K-edge. We confirmed that the local structures around In atoms of a $Ga_{1-x}In_xN$/GaN could be analyzed using XAFS system of SPring-8.

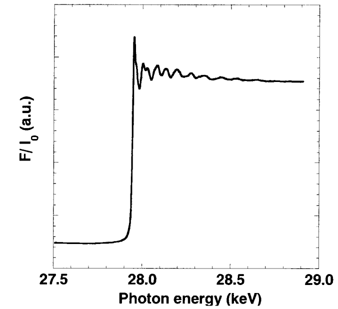

Fig.1 In K-edge fluorescence-yield spectrum of $Ga_{0.92}In_{0.08}N$/GaN single quantum well

References

[1] T. Miyajima, et al., SPring-8 User Experiment Report No.5 (2000A) 393.
[2] T. Miyajima, et al., SPring-8 User Experiment Report No.6 (2000B) 2.

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Investigation of local structure of Re active site of Re/γ–Fe_2O_3 catalysts by Re–K edge EXAFS

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Rhenium oxide supported on Fe_2O_3 has a unique property in the methanol selective oxidation reaction to produce methylal selectively. We measured Re K–edge EXAFS at BL01B1 to elucidate the local structure of rhenium species in ReO_x/γ-Fe_2O_3 and ReO_x/Al_2O_3.

The spectra were recorded at 8 K in a transmission mode. A Si(511) double crystal was used as monochromator and the X–ray intensities before and after sample were monitored by ionization chambers filled with pure Ar and Xe, respectively. The spectra were analyzed by the UWXAFS package. The phase shift and backscattering amplitude were calculated by the FEFF8 code and the coefficient of the multi-photon effects of rhenium cations was calculated from the EXAFS of rhenium oxides.

Figure 1 shows Fourier transformed Re K–edge EXAFS functions ($k^3\chi(k)$) of fresh ReO_x/γ-Fe_2O_3 and ReO_x/Al_2O_3 at various Re loadings. Phase shifts are not corrected in the figure.

In the spectra for low loaded ReO_x/γ-Fe_2O_3 (1.7 and 3.4 wt%), only Re–O contribution was observed at 0.175 nm and the contributions for longer distances such as Re–(O)–Re and Re–(O)–Fe were not observed. The Re–O distance and coordination number (CN) were not affected by the loading and were 0.175 nm and 4 in 1.7–9.2 wt%. This result together with the result of Re L_I edge XANES suggests that Re species on γ–Fe_2O_3 has tetrahedral ReO_4 structure regardless the Re loading. For ReO_x/γ-Fe_2O_3 (9.2 wt%), a Re–(O)–Fe contribution was observed at 0.384 nm with the CN of 1.0. The longer distance contribution cannot be fitted by a Re–O–Re contribution. This result together with the XRD result suggests that crystalline Re–Fe binary oxide was formed in ReO_x/γ-Fe_2O_3 (9.2 wt%). As the Re–O contribution was not affected by the loading, similar species to those at 9.2 wt% were expected to be formed at 1.7 and 3.4 wt%. The absence of the longer distance contributions at low loaded samples can be explained by a large statistical disorder.

For ReO_x/Al_2O_3 catalysts, on the contrary, Re–O contributions were affected by loading. at 1.0 wt% only Re=O was observed at 0.173 nm with CN being 2.9. A Re–O contribution was observed at 0.200 nm for ReO_x/Al_2O_3 2.0 wt% sample and the ratio of Re–O increased with increasing Re loading. In addition, longer distance contributions, which can be assigned to Re–(O)–Re contributions of ReO_2 were observed at 6.0 wt%. Thus, in the case of ReO_x/Al_2O_3, the local structure around Re is affected by loading. At low loading, Re exist as isolated species and at high loading Re exist as ReO_2.

We found that Re–Fe binary oxide was formed in ReO_x/γ-Fe_2O_3 catalysts. Such a binary oxide did not formed on ReO_x/Al_2O_3 catalysts. The formation of Re–Fe binary oxide can be a reason for high performance and long lifetime of ReO_x/γ-Fe_2O_3 catalysts.

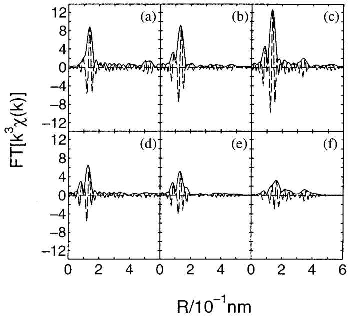

Figure 1. Fourier transformed Re–K edge EXAFS functions ($k^3\chi(k)$) of fresh ReO_x/γ-Fe_2O_3 (1.7 wt%) (a), ReO_x/γ-Fe_2O_3 (3.4 wt%) (b), ReO_x/γ-Fe_2O_3 (9.2 wt%) (c), ReO_x/Al_2O_3 (1.0 wt%) (d), ReO_x/Al_2O_3 (2.0 wt%) (e), and ReO_x/Al_2O_3 (9.2 wt%) (f).