XAFS analysis of optical activation process of Er in Si:Er_2O_3 thin film

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Introduction

Erbium-doped semiconductors which exhibit a sharp photoluminescence (PL) peak at a wavelength of ~1.54 μm arising from Er $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition, have great potential for realizing new optoelectronic devices. In this material, it is well known that oxygen enhances the Er-related PL. The identification of the local coordination of O around Er is one of the important factors contributing to the high PL efficiency. In this study, Er L_{III}-edge XAFS analysis is performed to investigate the optical activation process of Er in Si:Er_2O_3 thin film produced by the laser ablation method. The electronic modification is explained by a simple model based on a symmetrical variation of the local structure around Er.

Experiment

A KrF exicimer laser (λ = 248 nm) was used for ablating a 10 wt% Er_2O_3 bulk target prepared by a hot press technique from a Si and Er_2O_3 powder mixture. The substrate used in this study was a p-type (100)-oriented Si wafer. After Si:Er_2O_3 film deposition by laser ablation, the sample was annealed in N_2 ambient to activate the Er in the film. The annealing temperature and duration were 600℃ and 3 min, respectively. In XAFS experiments, a total-conversion He ion-yield (TCY) cell was used for current detection of He^+ ionized by photoelectrons ejected from the thin film.

Results and discussion

Figure 1 shows the Er L_{III}-edge XAFS spectra of (a) Er_2O_3 powder, (b) as-ablated Si:Er_2O_3 thin film, and (c) after annealing of (b). The Er L_{III}-absorption edge jumps are normalized to common values. The intensity of the white line caused by 2*p*-5*d* transition of thin films (b) and (c) is obviously stronger than that of (a) Er_2O_3. These results indicate that Er_2O_3 and Si:Er_2O_3 thin films differ in electronic configuration. In spite of these differences in XANES spectra, it was confirmed that EXAFS of the optically activated thin film was almost same as that of Er_2O_3 which had the sixfold coordination of O around Er.

The highest white line peak is obtained for the as-ablated sample: it is ~1.5 times higher than that of Er_2O_3. The white line peak intensity decreases after annealing, although it is still higher than that of Er_2O_3. In order to discuss the origin of the peak, the second derivative of the white line is performed. Although it is hard to distinguish the overlapping peaks in this original spectrum, the second derivative Er_2O_3 XANES is clearly split into a doublet, indicating that the resonant peak of Er_2O_3 originates from at least two electronic states. The second derivative of the as-ablated Si:Er_2O_3 thin film becomes a singlet. After annealing, a quasi-doublet with a small shoulder at the higher energy side is obtained; the electronic state is not one any longer.

The results of the peak height and the second-derivative analysis are explained by a simple model. First, the 5*d* state of Er_2O_3 is split into at least two electronic states. Assuming that the total density of states (DOS) of 5*d* is constant, the wide splitting of DOS reduces the absorption peak height of the 2*p*-5*d* transition. Laser ablation reconstructs the O local coordination around Er. If a higher symmetric local structure such as ErO_6 octahedron (O_h point group) is formed by the ablation, a concentrated DOS caused by the equivalent coordination of 6 O is produced. This higher DOS results in an intense, single absorption peak. After annealing, the O_h symmetry structure is considered to be slightly distorted. The DOS is not concentrated at a single energy in this structure, resulting in a quasi-doublet absorption peak.

The PL intensity of the as-ablated sample is two orders of magnitude lower than that of the annealed sample. The crystalfield may split the degenerated 4*f* orbits of Er, so that the forbidden Er $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition takes place. However, a higher order symmetry such as the ErO_6 octahedron may not produce a crystalfield to induce sufficient radiative transition. The symmetric distortion of the octahedron by annealing results in a suitable crystalfield for the strong PL.

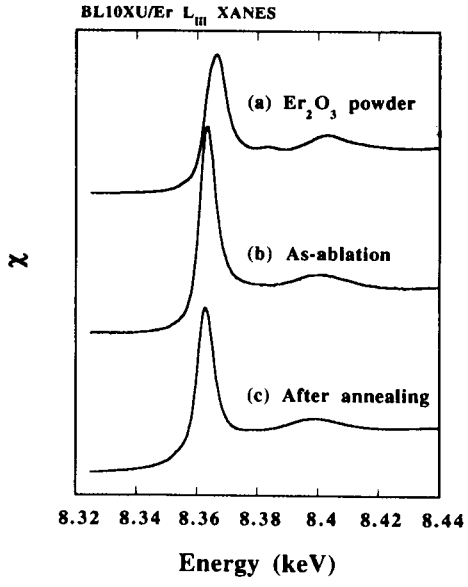

Figure 1 The Er L_{III}-edge XAFS spectra of (a) Er_2O_3 powder, (b) as-ablated Si:Er_2O_3 thin film, and (c) after annealing of (b).