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# Structural analyses of $Er^{3+}$-doped $Ga_2S_3$-$GeS_2$-$Sb_2S_3$ glasses by XAFS

Kohei KADONO*[1], Manabu ICHIKAWA[1], Kohei FUKUMI[2], Hiroyuki KAGEYAMA[2], Takashi WAKASUGI[1]

[1]Kyoto Institute of Technology, Sakyo-ku, Kyoto 606-8585, Japan

[2]National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan

## Introduction

Since $Ga_2S_3$-$GeS_2$-$Sb_2S_3$ glasses have properties of low phonon energy and high refractive index, wide transmission range, and high solubility of rare-earth ions, the glasses doped with rare-earth ions have received much attention for fluorescence materials in the near- and mid-infrared regions. Recently, we have investigated compositional dependences of spectroscopic properties for the $Er^{3+}$-doped $Ga_2S_3$-$GeS_2$-$Sb_2S_3$ glasses and have found that the component, $Ga_2S_3$, has large effects on the solubility and therefore the emission efficiency of the $Er^{3+}$ ions.

Here we report the XAFS studies on the network structure and coordination structure around $Er^{3+}$ ions for the glasses their compositional dependences.

## Experimental procedures

Undoped and Er-doped glasses were prepared by a conventional method for chalcogenide glasses from metal elements and sulfur as starting materials.

XAFS measurements were performed at PF BL-7C with Si (111) double crystal monochrometer in a transmission mode (Ga and Ge K-edges, and Sb $L_{III}$-edge) or a fluorescence mode (Er $L_{III}$-edge). Curve-fitting analyses were performed with the program REX2000 (Regaku Co.). Structural parameters of crystals, $Ga_2S_3$, $GeS_2$, $Sb_2S_3$, and $Er_2S_3$ were used as references.

## Results and Discussion

Table 1 summarizes the structural parameters around the network-forming cations in the glasses of various composition.

Table 1: Coordination numbers and bond distances (Å) between cation and sulfur obtained by XAFS analyses

| Composition* | Ga | | Ge | | Sb | |
|---|---|---|---|---|---|---|
| Ga-Ge-Sb | N | R | N | R | N | R |
| 30-40-30 | 4.4 | 2.32 | 3.8 | 2.20 | 4.9 | 2.53 |
| 20-50-30 | 4.7 | 2.31 | 3.9 | 2.20 | 4.3 | 2.53 |
| 10-60-30 | 4.3 | 2.31 | 3.4 | 2.20 | 3.6 | 2.52 |
| 0-70-30 | | | 3.4 | 2.20 | 4.7 | 2.52 |
| 30-50-20 | 4.3 | 2.32 | 3.3 | 2.20 | 6.3 | 2.51 |
| 10-50-40 | 4.8 | 2.32 | 4.0 | 2.20 | 5.3 | 2.52 |
| 0-50-50 | | | 3.7 | 2.20 | 5.0 | 2.52 |
| Crystals | 4 | 2.32 | 4 | 2.19 | 4 | 2.61 |

*Glass compositions are described as cation mol%.

The average coordination numbers around Ga and Ge were 4.5 and 3.6, respectively. These values were almost the same as those of the crystals, $Ga_2S_3$ and $GeS_2$. On the other hand, the average coordination number around Sb was 4.8 which was slightly larger than that of the $Sb_2S_3$ crystal. The bond distances of Ga-S and Ge-S in the glasses were also the same as those of the crystals while the Sb-S distance was slightly shorter than that of the $Sb_2S_3$ crystal. The structure of the glasses has been also investigated by means of Raman spectroscopy which suggested that the glass network consists of $GaS_4$ and $GeS_4$ tetrahedra, and $SbS_3$ pyramidal units. Although both results on the structures around Ga and Ge are rather consistent, further investigation is necessary.

Figure 1 shows Fourier transforms of the XAFS functions at Er $L_{III}$-edge for various glass compositions. The structural parameters obtained by the curve-fittings were presented in Table 2. The coordination number around the Er ion was about 7 and the Er-S bond distance was 2.80 Å. The coordination structure was hardly varied with the glass composition.

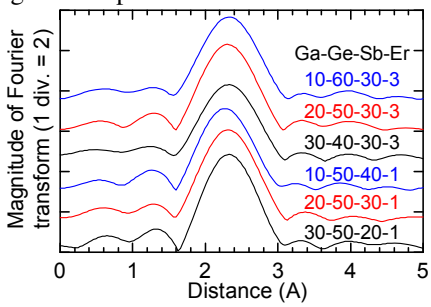


Fig. 1. Fourier transforms of XAFS functions at Er $L_{III}$-edge for glasses of various compositions.

Table 2: Coordination structure around Er ions

| Ga-Ge-Sb-Er | N | R (Å) | DW (Å) |
|---|---|---|---|
| 10-60-30-3 | 7.3 | 2.80 | 0.104 |
| 20-50-30-3 | 6.4 | 2.80 | 0.093 |
| 30-40-30-3 | 6.6 | 2.79 | 0.105 |
| 10-50-40-1 | 6.9 | 2.80 | 0.104 |
| 20-50-30-1 | 7.3 | 2.81 | 0.097 |
| 30-50-20-1 | 6.7 | 2.81 | 0.086 |
| $Er_2S_3$ crystal | 6.5 | 2.73 | 0.102 |

## References

[1] V. Moizan, et al., Opt. Mater. 31, 39 (2008).

* kadono@kit.ac.jp