## §2. Characterization of Erbium Oxide Coatings by Cathodoluminescence Measurements

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The development of an  $Er_2O_3$  ceramic coating has been conducted for reduction of the MHD pressure drop in the Li cooled blanket system and also for tritium permeation barrier in the Flibe or LiPb cooled blanket systems. Recently, applications of the metal organic CVD (MO-CVD) method in gas phase and the metal organic decomposition (MOD) method in liquid phase have been studied for fabrication of large area coatings on blanket components. The crystallinities of the  $Er_2O_3$  coatings fabricated by the MO-CVD and MOD methods have been examined by cathodoluminescence measurements.

For understanding the results of the optical characterizations, theoretical studies have been performed on relations between optical properties and crystal structures of  $\text{Er}_2\text{O}_3$ . In order to obtain the theoretical transition spectra of  $\text{Er}^{3+}$  ion at the other two occupied sites in  $\text{Er}_2\text{O}_3$ , multiplet energy levels and absorption spectra were calculated by relativistic first-principles many-electron calculation (DVME method).<sup>1)</sup> The cluster models used were constructed on the basis of the crystal structure of  $\text{Er}_2\text{O}_3$  at room temperature. And, the change in the theoretical transition spectra with calculated model structures that include the distortion around defects are also studied.

Figure 1 shows the cathodoluminescence spectra of  $Er_2O_3$  coatings fabricated by the MO-CVD method. The thicknesses of the coatings were 0.3-0.6 µm and the spectra were measured under irradiations of 10-12 keV electron beams at room temperature. The significant deference between the spectra is the luminescence intensities in the



Fig. 1 Cathodoluminescnce spectra of  $Er_2O_3$  coatings fabricated with the MO-CVD method.

640-690 nm band increasing with the substrate temperature in the fabrication process. Peak width measurements in Xray diffraction patterns indicate that the crystallinity of the coating could be improved significantly with the substrate temperature in the range of 450-600 °C. Similar relations of the luminescence intensities in the 640-690 nm band and the peak widths of the X-ray diffraction patterns with the substrate temperature in the fabrication process were observed also for the Er<sub>2</sub>O<sub>3</sub> coatings fabricated by the MOD method. Luminescence intensity in the 640-690 nm band is considered to be sensitive especially to the crystallinity of the Er<sub>2</sub>O<sub>3</sub> coating. The relation between the luminescence spectra and the crystallinities would be effective for nondestructive inspections and analyses of the large area Er<sub>2</sub>O<sub>3</sub> coating on blanket components.

Figure 2 (a) and (b) show theoretical absorption spectra calculated with the cluster models based on the structure around the 24d site and 8a site in  $Er_2O_3$ , respectively. Since  $Er^{3+}$  ion at 24*d* site is in  $C_2$  symmetry, the absorption from  $4f^{11}-4f^{11}$  transition has intensity (dashed line). Absorption intensity and wavelength slightly changed in case of model considering the distortion with displacement of one oxygen ion (thin and heavy solid line). On the other hand, because  $Er^{3+}$  ion at 8a site is in  $S_6$ symmetry includes point symmetry, the transition is the forbidden transition and calculated absorption intensity has no value. But in case of the model considering the break of symmetry with the distortion, calculated intensity has value (Fig. 2(b)). The results indicate that  $Er^{3+}$  ion at 8*a* site may contribute to the absorption intensity if the structure was distorted with defects.

1) Ogasawara, K. et al. : Phys. Rev. B 64 (2001) 115413

