

XAFS investigations of nanocrystalline Eu-doped BaAl₂O₄

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Introduction

Alkaline earth aluminates are promising starting compounds for the preparation of fluorescent and phosphorescent doped materials. The room-temperature (RT) phase of BaAl₂O₄ becomes a luminescent material with emission in the red or blue-green spectral range when doped with Eu³⁺ or Eu²⁺ ions, respectively. Here we investigate the influence of europium doping on the structure of BaAl₂O₄ by means of X-ray absorption fine structure spectroscopy (XAFS) at RT. This system is of particular interest because of its excellent optical properties. The quite complicated crystal structure of the host material (hexagonal system, space group *P6₃*) with several possible lattice sites for the Eu dopant, as well with several possible interstitial sites for oxygen, makes XAFS an ideal tool to determine the coordination around Eu and its position within the host lattice.

Methods

Nanosized powder samples of pure BaAl₂O₄ and one doped with 4.9 at.% Eu in relation to Ba were prepared from Ba(NO₃)₂, Al(NO₃)₃·9H₂O, and Eu(NO₃)₃·6H₂O using a hydrothermal route followed by a thermal treatment at 1100 °C for 4h. For the XAFS studies, the powder samples were diluted with BN and dispersed on self-adhesive kapton tapes. Several tapes were stacked in order to obtain an absorption suited for XAFS measurements, which were carried out at both the Ba and the Eu L₃-edges on beamline BL10 at the Dortmund Electron Accelerator DELTA using a channel-cut Si(111) monochromator and gas-filled ionization chambers as detectors.

Results and discussion

EXAFS studies at the Ba L₃-edge for both samples, pure and Eu-doped BaAl₂O₄, gave evidence that the structure of the doped sample was very similar to that of pure BaAl₂O₄. The determined Ba-O and Ba-Al distances in these samples agree well with those obtained by a Rietveld structure refinement using the X-ray diffraction patterns for both samples. XANES measurements at the L₃-edge of the Eu doped sample clearly revealed the presence of solely Eu³⁺ ions, but the radial distribution function resulting from the EXAFS data was completely different from those for the investigated reference phases Eu₂O₃ and AlEuO₃. Impurity phases containing Eu were not detected, so the incorporation of the Eu³⁺ dopant on a regular lattice site of the BaAl₂O₄ host is very likely. We tested several possible lattice sites in the course of the Eu-EXAFS data fitting. Replacement of Ba²⁺ ions on the regular Ba2 site by Eu³⁺ ions, and including an additional oxygen into the lattice for charge compensation, gave the best results.

Conclusions

EXAFS investigations have shown that Eu-doping in BaAl₂O₄ leads to substitution of Eu³⁺ ions for Ba²⁺ on the Ba2 site in the host structure, with charge compensation by an interstitial oxygen in the vicinity of the related Ba2 site. The presence of any impurity phase could be excluded.