CRYSTAL AND TWIN STRUCTURES OF THE ZrO_2:Sc_2O_3 CRYSTALS

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An increasing interest in electrolyte materials for advanced energy applications demands investigation of their real structure and its influence on the physical properties. It is relevant to investigate the crystal and twin structures of electrolytes, for which the considered properties depend on domain walls distribution [1]. ZrO_2 doped with Sc is considered as prospective solid electrolyte for application in solid oxide fuel cells (SOFCs).

The present work is devoted to structure investigation of ZrO_2 doped by Sc_2O_3 (10 mol.%) (ZSO-10) and determination the twin structure in trigonal phase of the ZSO-10 crystal in a wide temperature range of 300-1253 K.

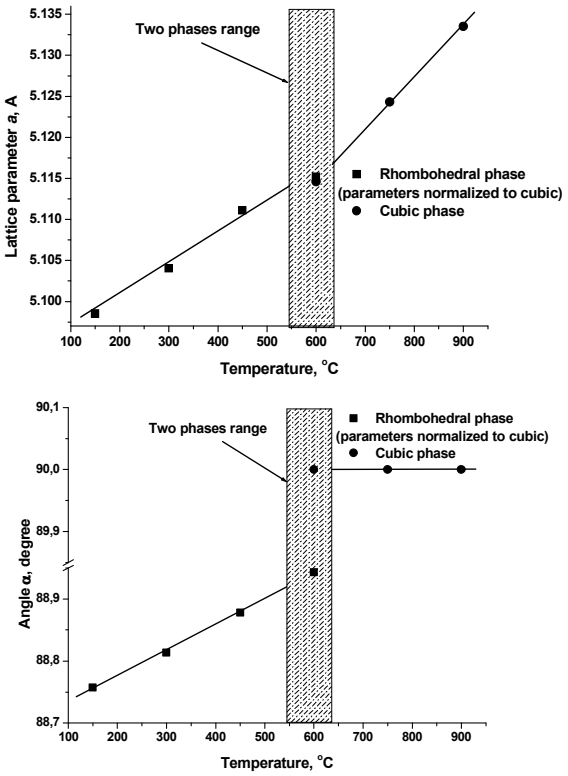

Figure 1. Temperature dependencies of the lattice parameters of ZSO-10. Parameters of the rhombohedral cell are normalized to the cubic ones.

In order to study the thermal behavior of the crystal structure of ZrO_2:Sc_2O_3 the structure investigations were carried out at a powder diffractometer at beamline B2 (HASYLAB/DESY). High-temperature diffraction data were collected in the Debye-Scherrer capillary geometry using the on-site readable image plate detector OBI and STOE furnace. Data analysis was carried out by the Rietveld method using the WinCSD program package. Determination of domains orientations was performed using the Laue method. The white beam synchrotron experiments have been carried out using the Kappa-diffractometer at HASYLAB beamline F1 equipped with MAR CCD system and a gas-stream heating device.

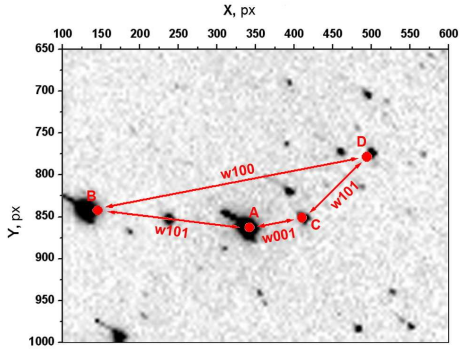

Figure 2. A section of Laue pattern collected at a CCD-sample distance of 300.4 mm and calculated spot positions for observed twin laws (with respect to reference domain *A*).

The powder diffraction examination revealed that rhombohedral structure (space group $R\bar{3}$) of ZSO-10 transforms into high-temperature cubic structure (space group $Fm\bar{3}m$) at 873 K. Temperature dependencies of the lattice parameters are presented in Fig. 1.

Analysis of Laue patterns collected at room temperature confirms that the ZSO-10 crystal was twinned relatively to intersecting (101) and (100)/(001) mirror planes in the rhombohedral phase (Fig. 2).

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References

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