P-17

Crystal structure and defect structure of selected $Ca_9RE(VO_4)_7$ single crystals: A high-resolution diffraction, white beam topography and powder diffraction study

A. Behrooz[1]*, W. Paszkowicz[1], P. Romanowski[1], B. Nazarenko[2], A. Shekhovtsov[2], W. Wierzchowski[3], K. Wieteska[4] and C. Paulmann[5]

[1]*Institute of Physics, Polish Academy of Sciences, al. Lotnikow 32/46, PL-02668 Warsaw, Poland,*
[2]*Institute for Single Crystals, NAS of Ukraine, Lenin Ave. 60, 61001, Kharkov, Ukraine*
[3]*Institute of Electronic Materials Technology (ITME), Wólczyńska 133, Warszawa 01-919, Poland*
[4]*National Centre for Nuclear Research, Radioisotope Centre POLATOM (NCNR), Andrzeja Soltana 7, Otwock-Świerk 05-400, Poland*
[5]*HASYLAB at DESY, 85, Notkestr., Hamburg 22607, Germany*

Keywords: calcium rare earth vanadate, structure refinement

*e-mail: behrooz@ifpan.edu.pl

Compounds of $Ca_9RE(VO_4)_7$ formula (RE = a rare earth) are structurally closely related to whitlockite mineral, $Ca_9(MgFe)(PO_4)_6PO_3OH$. Such materials are considered for applications in optoelectronics, e.g., in white-light emitting diodes, as discussed in Refs. [1, 2]. Compounds of $Ca_9RE(VO_4)_7$ structure (space group $R3c$) accommodate the RE atoms in Ca sites by assigning a partial occupancy of Ca and RE atoms [3, 4]. The current survey, extracts some basic information on structure and quality of $Ca_9RE(VO_4)_7$ (R = La, Nd, Gd) single crystals with the use of high-resolution diffraction, white beam topography and powder diffraction.

$Ca_9RE(VO_4)_7$ single crystals were grown by the Czochralski method. Phase analysis has shown that the crystals are pure $Ca_9RE(VO_4)_7$ phases. The results of Rietveld refinements are compared with literature data for polycrystalline samples prepared by solid state reaction [3, 4]. Small discrepancies in lattice parameter values are attributed to minor excess from stoichiometry of the single crystal studied. X-ray rocking curves and reciprocal space maps were established using a laboratory high-resolution diffractometer. Topographs have been obtained in reflection geometry using white beam at a synchrotron beamline. A comparison among the results of all applied approaches shows that the studied crystals reveal specific similarities and differences in the defect structure. The rocking curves as well as the reciprocal space maps of symmetrical 0 0 30 and asymmetrical 1 0 16 reflections prove that the crystals are generally of good quality and display the defects characteristic for the given crystal, such as dislocations, point defects and mosaics. The analysis of the topographs clarifies the existence of dislocations and/or small inclusions in the $Ca_9La(VO_4)_7$ and $Ca_9Nd(VO_4)_7$ single crystals and the incoherent inclusions in the $Ca_9Gd(VO_4)_7$ single crystal.

[1] X. Wu, Y. Huang, H.J. Seo, *Ceramics Int.* **37** (2011) 2323.
[2] L. Liu, R.-J. Xie, N. Hirosaki, Y. Li, *J. Spectrosc. Dyn*. **3**, (2013) 1.
[3] A. A. Belik, V. A. Morozov, R. N. Kotov, S. S. Khasanov, B.I. Lazoryak, *Crystallogr. Rep*. **42** (1997) 751.
[4] A. A. Belik, V. A. Morozov, S. V. Grechkin, S. S. Khasanov, B. I. Lazoryak, *Crystallogr. Rep*. **45** (2000) 798.