Structural analysis of metavanadate phosphors AVO_3 (A: K, Rb and Cs)

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Metavanadate phosphors AVO_3 (A: K, Rb and Cs) were first discovered by Gobrecht *et al*. in 1957 [1]. The AVO_3 shows a broad-band emission at 380 – 700 nm. We have measured quantum efficiencies (η) of these compounds; the η of KVO_3, $RbVO_3$ and $CsVO_3$ were 4, 59 and 80%, respectively. The origin of intense luminesecence of the $CsVO_3$ has not been disccussed well in spite of its remarkable high value of η. In this work, we have studied the powder neutron diffraction for understanding luminescent properties of the AVO_3 from the viewpoint of the structural features.

The polycrystalline samples of AVO_3 (A: K, Rb and Cs) were prepared by a solid state reaction. The powder neutron diffraction measurements for the obtained powder samples were performed using the HERMES spectrometer installed at the research reactor JRR-3M in Japan Atomic Energy Agency, Tokai, Japan [2]. The wavelength of the incident neutron was selected to be 1.8265 Å. The diffraction data were collected in the 2θ range from 3 to 153 deg. in the step interval of 0.05 deg. at room temperature. The obtained data analyzed by the Rietveld method using a computer program RIETAN-FP [3].

Structural analysis of $CsVO_3$ was carried out by using a reported structural model, space group *Pbcm* [4]. The structural parameters were refined as follows: a = 5.3979(3) Å, b = 12.2553(8) Å and c = 5.7881(3) Å. The reliability factors were R_{wp} = 4.97%, R_e = 2.37%, R_I = 2.89% and R_F = 1.54%. Main diffraction peaks were almost fitted with the calculation result, however, the minor diffraction peaks can not be indexed by this structural model. In the KVO_3 and $RbVO_3$, the structural analyses were also carried out, and the some minor peaks were not indexed with *Pbcm* as similar with the case of $CsVO_3$.

For the discussion of luminescent properties of the AVO_3, the structural distortion should be correctly determined, because the emission intensity in these compounds could strongly depend on the distortion of the VO_4 tetrahedra in the crystal structure. In the conventional structural analysis using X-ray diffraction [4], the structural analysis of AVO_3 was carried out using the space group *Pbcm*, and clear differences were not observed among the VO_4 tetrahedra of the AVO_3 (A: K, Rb and Cs). Therefore, unindexed peaks in this neutron diffraction is expected to be a key point for the discussion of the origin for luminescent property of the AVO_3. The detailed structural analysis of these compounds are in progress.

References

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