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 ($\eta$) of these compounds; the $\eta$ of KVO$_3$, RbVO$_3$ and CsVO$_3$ were 4, 59 and 80%, respectively. The origin of intense luminescence of the CsVO$_3$ has not been discussed well in spite of its remarkable high value of $\eta$. 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 2$\theta$ 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 simi-

References