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# The Luminescence of The Phosphor $Sr_2ZrO_4$ with One-dimensional Chains Structure

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**Abstract:** A new type of phosphor $Sr_2ZrO_4$ with one-dimensional structure was prepared by solid reaction and its luminescence is seen at room temperature. The excitation and emission spectra were measured and display broad maximum at 354 nm and 386 nm respectively. The mechanism of this luminescence is ascribed to charge transfer.

**Keyword:** Luminescence, zirconate, one-dimensional structure.

## Introduction

The number of zirconates which can be excited by conventional UV excitation ($\lambda$>240 nm) is small, so that zirconate emission is easily overlooked. Some compounds which absorb coventional UV radiation, *eg*. $ZrO_2$ and $BaZrO_3$ (240 nm) do not luminence owing to energy migration[1]. On the other hand, although several zircinates such as $ZrP_2O_7$[2], $BaZrSi_3O_9$[3] and $SrZrSi_2O_7$[4] show efficient UV zirconate emission (around 300 nm), their excitation wavelengths are shorter than usual (200 nm). Moreover, their luminescence are at very low temperature (4.2K), which limits their applications. However, we found that zirconate can show efficient luminescence if there is one-dimensional structure in the crystal structure of zirconates. For example, because $Ca_3ZrSi_2O_9$[1] contains pairs of edge-sharing zirconate octahedral, although this is not real low-dimensional structure, it shows a yellow photoluminescence.

In our previous paper[5], several rules about luminescence of one-dimension structure have been advanced. In this work, a new type of phosphor $Sr_2ZrO_4$ with one-dimensional chains was prepared under direction of these rules. Compared to the luminescence of those Zr compounds, that of $Sr_2ZrO_4$ is at room temperature and its intensity is much higher than those. Particularly, its excited wavelength lies in the longer wavelength (354 nm) which is available on conventional instrumentation.

## Experimental

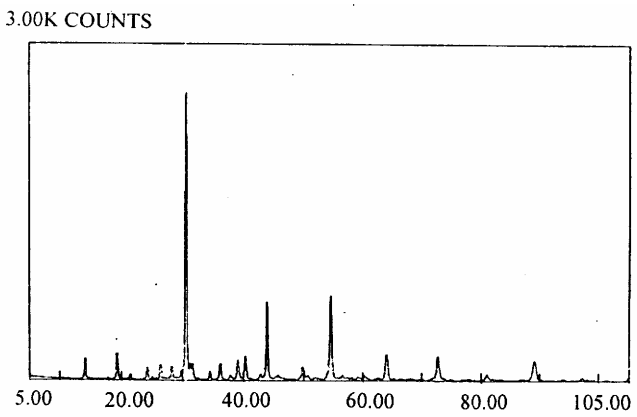
Powder samples were prepared from AR $SrCO_3$, AR $ZrO_2$ by heating at 1200℃ in the air for 18 hours with two intergrinds. They were checked by X-ray diffraction (CuK$\alpha$ radiation.).

The luminescence measurements were performed using a HITACHI MPF-4 fluorescence spectrophotometer equipped with xenon lamp.

**Results and Discussion**

The composition $Sr_2ZrO_4$ has been reported[6,7] to be in the tetragonal crystal system in space group I4/mmm with all parameters a=4.103, c=12.82 and have $K_2NiF_4$ structure. It is well known that a number of compounds like $K_2NiF_4$ possess low-dimensional structure. Moreover, we can find that the x-ray diffraction of $Sr_2ZrO_4$ (see **Figure 1**) is almost the same as that of $Sr_2CeO_4$[8] (see **Figure 2**), another kind of compound containing one-dimensional structure. So we conclude the structure of $Sr_2ZrO_4$ contains one-dimensional chain structure. The crystal structure of $Sr_2ZrO_4$ is given in **Figure 3**. The chain structure is formed by $ZrO_6$ edge-sharing octahedral and there are two *trans* terminal Zr-O groups perpendicular to the plane defined by four equatorial $\mu^2$-O atoms in the chains.

**Figure 1** The X-ray spectra of $Sr_2ZrO_4$




The excitation and emission spectra of sample are given in **Figure 4** and display broad maximum at 354 nm and 386 nm, respectively. The mechanism of luminescence is based on ligend-to-metal change transfer from $O^{2-}$ to $Zr^{4+}$. Because a relatively electron-rich terminal O atom is bound to a single oxidizing $Zr^{4+}$, when the terminal O atom absorbed the outside energy, an electron of outer orbit of O atom can transfer to the orbit of $Zr^{4+}$, forming the CT state (with $O^-$---$Zr^{3+}$ characteristics). When this electron transfer to the lower energy state of $Zr^{4+}$ occurs, photon is radiated.

**Figure 2** The X-ray spectra of $Sr_2CeO_4$

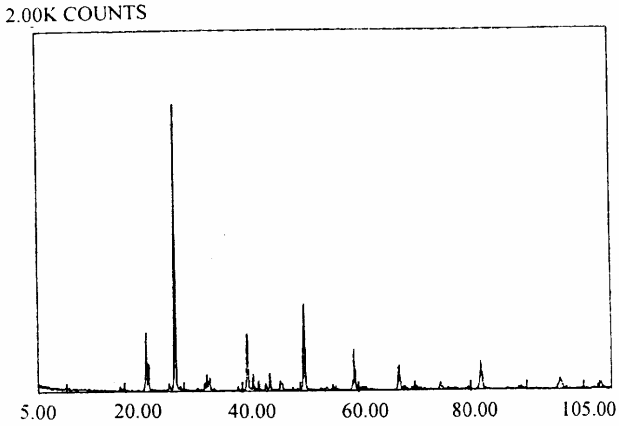



**Figure 3** The crystal structure of $Sr_2ZrO_4$

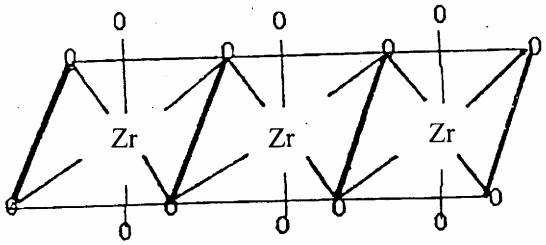
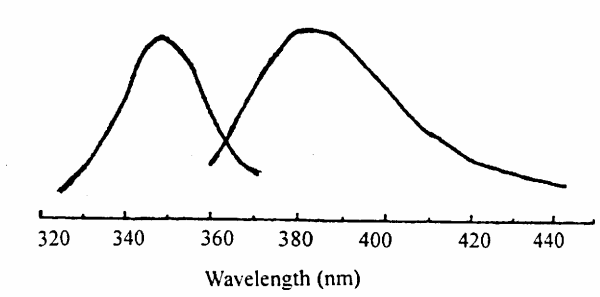



**Figure 4** The excitation and emission spectra of $Sr_2ZrO_4$




## Conclusion

We believe that the low-dimensional structure is very important to some luminescent materials. The other luminescence of Zr compound is too weak to be seen at room temperature. The reason is the tetrahedra of $Zr^{4+}$ in the host lattice are isolated

from each other, while in the case of $Sr_2ZrO_4$, when they share oxygen ion and form linear chain structure, efficient luminescence appears. If we could utilize the characteristics we would discover more and more new phosphors, for instance, $Sn^{4+}$, $Ti^{4+}$, $Hf^{4+}$, $Ce^{4+}$ and *etc*.

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