

## Phase analysis of Zr doped $\text{UO}_2$

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### 1. Introduction

In a hypothetical case of a nuclear reactor severe accident, the reactor core could melt and form a mixture (called corium) of  $\text{UO}_2$ ,  $\text{ZrO}_2$  and other elements. Therefore, a characterization of the corium is needed. For this purpose, XRD analyses for molten simulated corium samples have been performed [1-3].

In this study, the phases of the  $\text{UO}_2$  -  $\text{ZrO}_2$  mixture sintered at high temperature and its oxidized sample were investigated by X-ray diffraction for a basic phase study.

### 2. Experimental and Results

#### 2.1 Sample preparation

The sintered pellets were prepared with the composition of 0, 5 and 25 at% - Zr in  $\text{UO}_2$ - $\text{ZrO}_2$  mixture by heating for 12 h at 1700 °C in an atmosphere of  $\text{H}_2$ . The oxidized samples of the solid solutions were prepared by a heating from a room temperature to 500 °C with a velocity of 1 °C / min. in air.

#### 2.2 XRD system

The X-ray diffraction system (D5000, SIEMENS) with a  $\text{CuK}_\alpha$  line filtered through a Ni foil was used to obtain XRD patterns of the sintered  $\text{UO}_2$ - $\text{ZrO}_2$  samples and the oxidized  $\text{UO}_2$ - $\text{ZrO}_2$  solid solution samples. The measurement was carried out with a scanning step of 0.02° for 1s per each count and a divergence slit of 1 mm and a detector slit of 0.1 mm in width. The X-ray beam current was 40 mA at a 40 kV beam generation power.

#### 2.3 XRD spectrum of the sample sintered at 1700 °C

The XRD patterns of the  $\text{UO}_2$ - $\text{ZrO}_2$  samples sintered at high temperature with the composition of 0, 5 and 25 at% - Zr are shown in Fig. 1. The pure  $\text{UO}_2$  has a cubic phase and showed a value of  $a = 5.464 \text{ \AA}$ . In XRD pattern of the sample of 5 at% - Zr, cubic phase of  $\text{UO}_2$  sample was maintained but the peaks were shifted to the high degrees( $2\theta$ ). Therefore, the size of its unit cell was reduced and the lattice parameter showed a value of  $a = 5.430$ . In case of the sample of 25 at% - Zr, the value of  $a$

= 5.377 was obtained. In the result, the increase of the composition of Zr solute into the  $\text{UO}_2$  lattice decreases the volume of the  $\text{UO}_2$  unit cell without a change of the cubic phase.

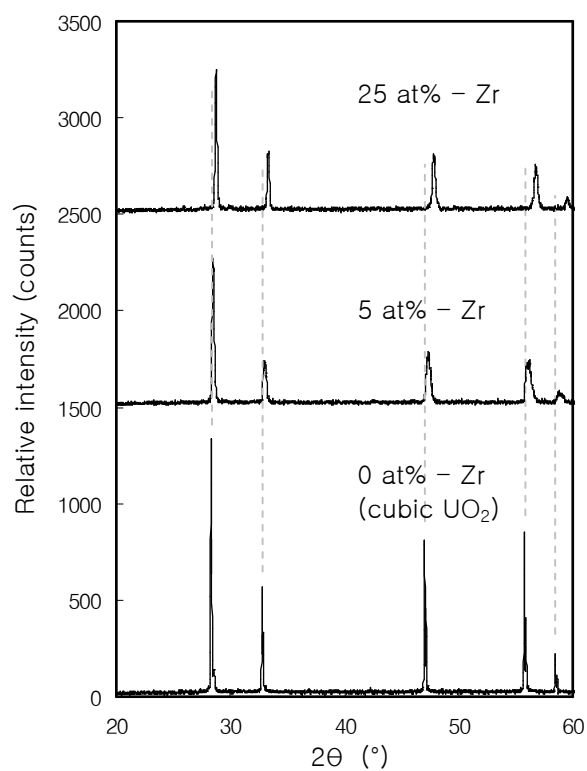


Figure 1. XRD patterns of the sintered  $\text{UO}_2$ - $\text{ZrO}_2$  samples with the composition of 0, 5, 25 at% - Zr

#### 2.4 XRD spectrum of the oxidized sample of solid solution

The XRD patterns of the oxidized samples of the  $\text{UO}_2$ - $\text{ZrO}_2$  solid solutions as stated above are shown in Fig. 2. The  $\text{UO}_2$  sample with 5 at% - Zr was oxidized to  $\text{U}_3\text{O}_8$  of the orthorhombic phase. On the other side, the  $\text{UO}_2$  with 25 at% - Zr was oxidized to  $\text{U}_3\text{O}_8$  of the hexagonal phase, and  $\text{ZrO}_2$  of tetragonal phase not monoclinic that the pure

ZrO<sub>2</sub> has a monoclinic phase in general was shown in XRD spectrum.

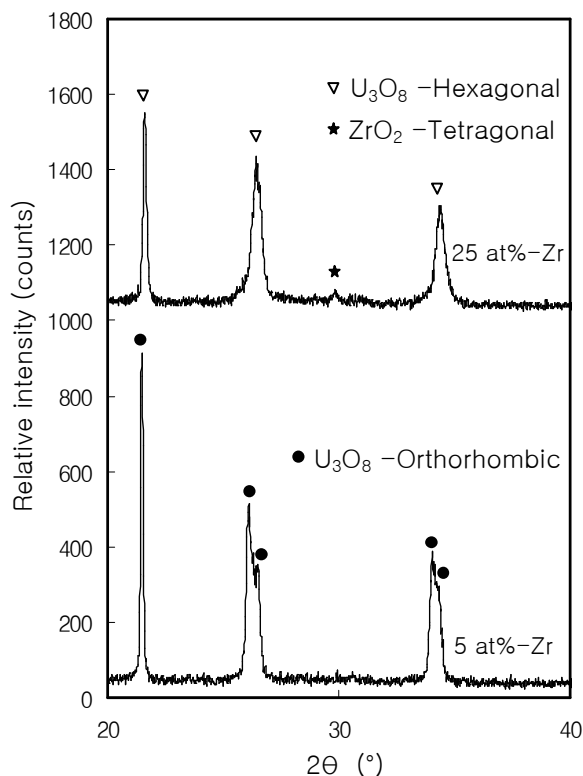


Figure 2. XRD patterns of the oxidized UO<sub>2</sub>-ZrO<sub>2</sub> solid solution samples with the composition of 5, 25 at% - Zr

### 3. Conclusion

It was identified that ZrO<sub>2</sub> was soluted into the lattice of a cubic phase of UO<sub>2</sub> and contracted the size of the unit cell. And, in the oxidation of the solid solution sample, the UO<sub>2</sub> was oxidized to U<sub>3</sub>O<sub>8</sub> of the hexagonal phase not orthorhombic due to the solute ZrO<sub>2</sub>.

We are planning to analyze the phases by an XRD for samples with various composition of Zr for a basic phase study about corium.

### REFERENCES

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