## Metal-substitution effects in temperature- and pressure-induced phase transitions of long-term heat-storage ceramics λ-Ti<sub>3</sub>O<sub>5</sub>

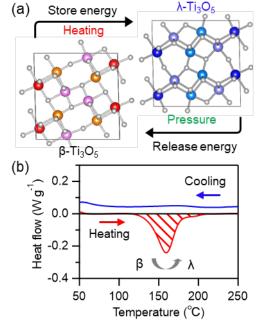
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To achieve carbon-neutral, it is crucial not only to promote renewable energy but also to efficiently use the energy produced. Especially, effective reuse of wasted heat energy is an urgent issue. From this point of view, long-term heat-storage ceramics, lambda-trititanium-pentoxide ( $\lambda$ -Ti<sub>3</sub>O<sub>5</sub>) is one of the promising materials.  $^1\lambda$ -Ti<sub>3</sub>O<sub>5</sub> is a metastable phase of Ti<sub>3</sub>O<sub>5</sub> discovered in 2010 by our group. Since this material has bistability with the energetically most stable  $\beta$ -Ti<sub>3</sub>O<sub>5</sub>, it shows reversible phase transition between  $\lambda$  and  $\beta$ -phases in response to pressure and heat. The stored thermal energy can be released at a desired timing by applying pressure. Furthermore, the heat storage performance can be adjusted by metal substitution of

the Ti atom.<sup>3-6</sup> In this presentation, we report the synthesis of Sc-substituted  $\lambda$ -Ti<sub>3</sub>O<sub>5</sub> by coprecipitation method and long-term heat-storage property of the obtained material.

Sc-substituted  $\lambda$ -Ti<sub>3</sub>O<sub>5</sub> was synthesized by sintering rutile-TiO<sub>2</sub> precursor coated with Sc(OH)<sub>3</sub> in a reductive atmosphere. Powder X-ray diffraction (PXRD) measurement showed that the  $\lambda$ -phase was obtained as the major phase. Elemental analysis showed that the chemical formula is Sc<sub>0.054</sub>Ti<sub>2.946</sub>O<sub>5</sub>. The phase transition pressure at which half of the  $\lambda$ -phase changes to  $\beta$ phase was determined as 350 MPa from the PXRD patterns after pressurizing the sample uniaxially. The heat-storage property was measured by differential scanning calorimetry (DSC) using the pressure-produced β-phase sample by applying 600 MPa. The phase transition temperature from βphase to λ-phase was decreased from 197°C of λ- $Ti_3O_5$  to 158 °C of  $\lambda$ -Sc<sub>0.054</sub> $Ti_{2.946}O_5$ .



**Figure 1.** (a) Crystal structure of  $\lambda$ - and  $\beta$ - Ti<sub>3</sub>O<sub>5</sub> and schematic illustration of long-term heat-storage. (b) Endothermic peak of  $\lambda$ -Sc<sub>0.054</sub>Ti<sub>2.946</sub>O<sub>5</sub> observed using DSC.

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