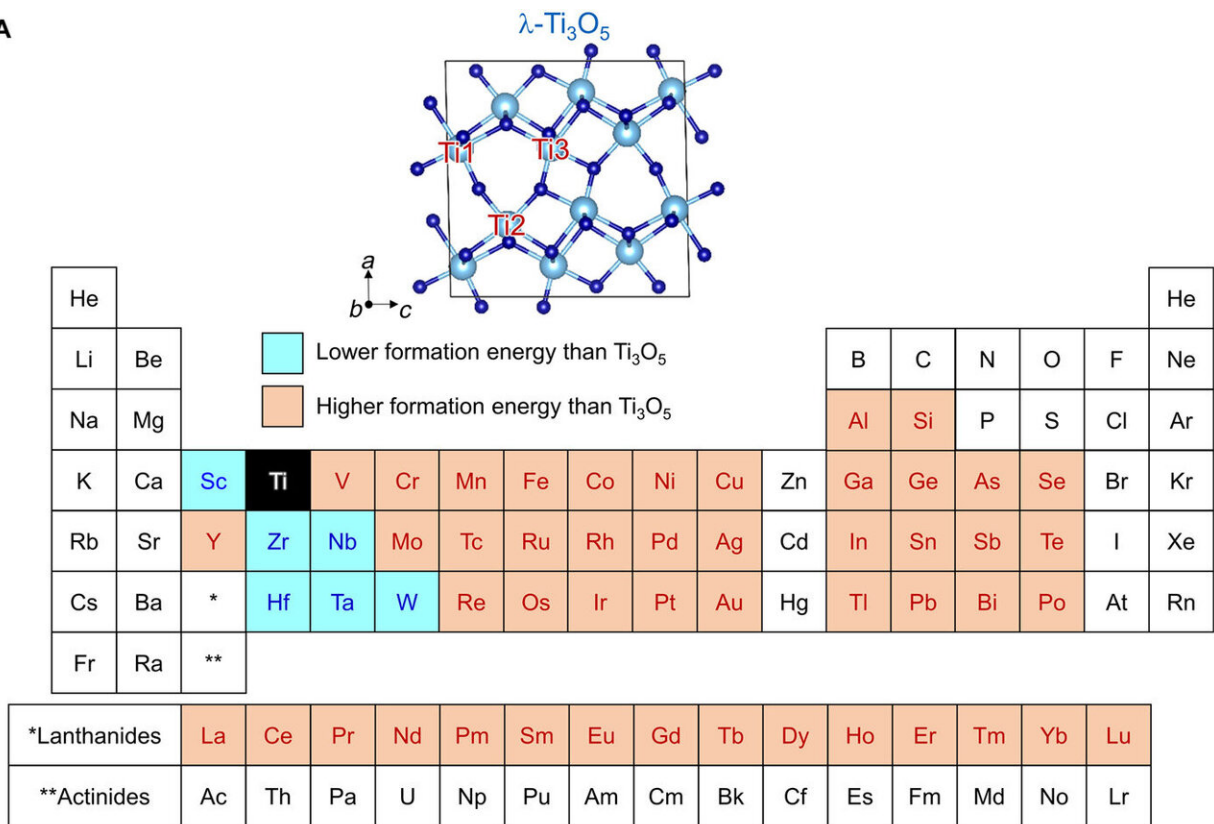


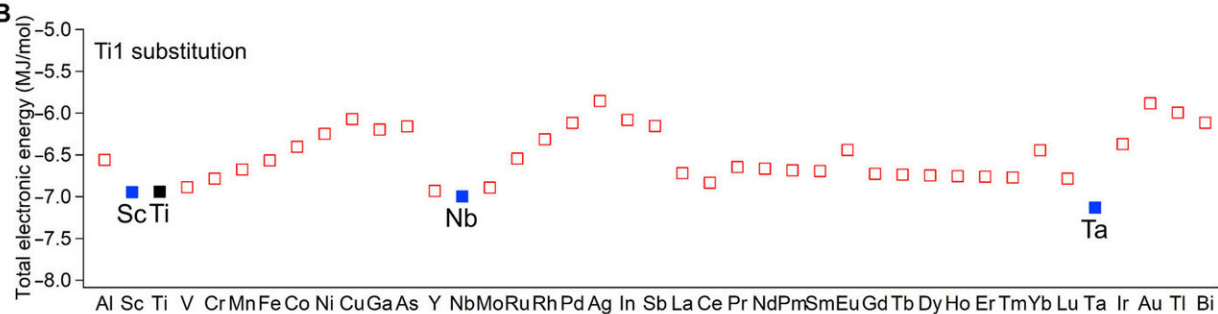
Long-term heat-storage ceramics absorbing thermal energy from hot water

July 13 2020, by Thamarasee Jeewandara

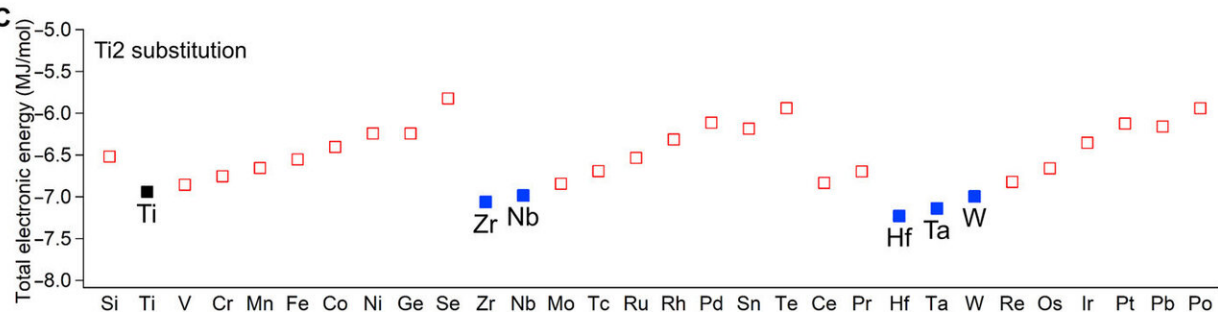
A



B



C



First-principles calculations of formation energies. (A) Periodic table colored by the total electronic energies of $\lambda\text{-Ti}_3\text{O}_5$ with an elemental substitution. Blue elements are those where substituted $\lambda\text{-Ti}_3\text{O}_5$ shows a lower formation energy

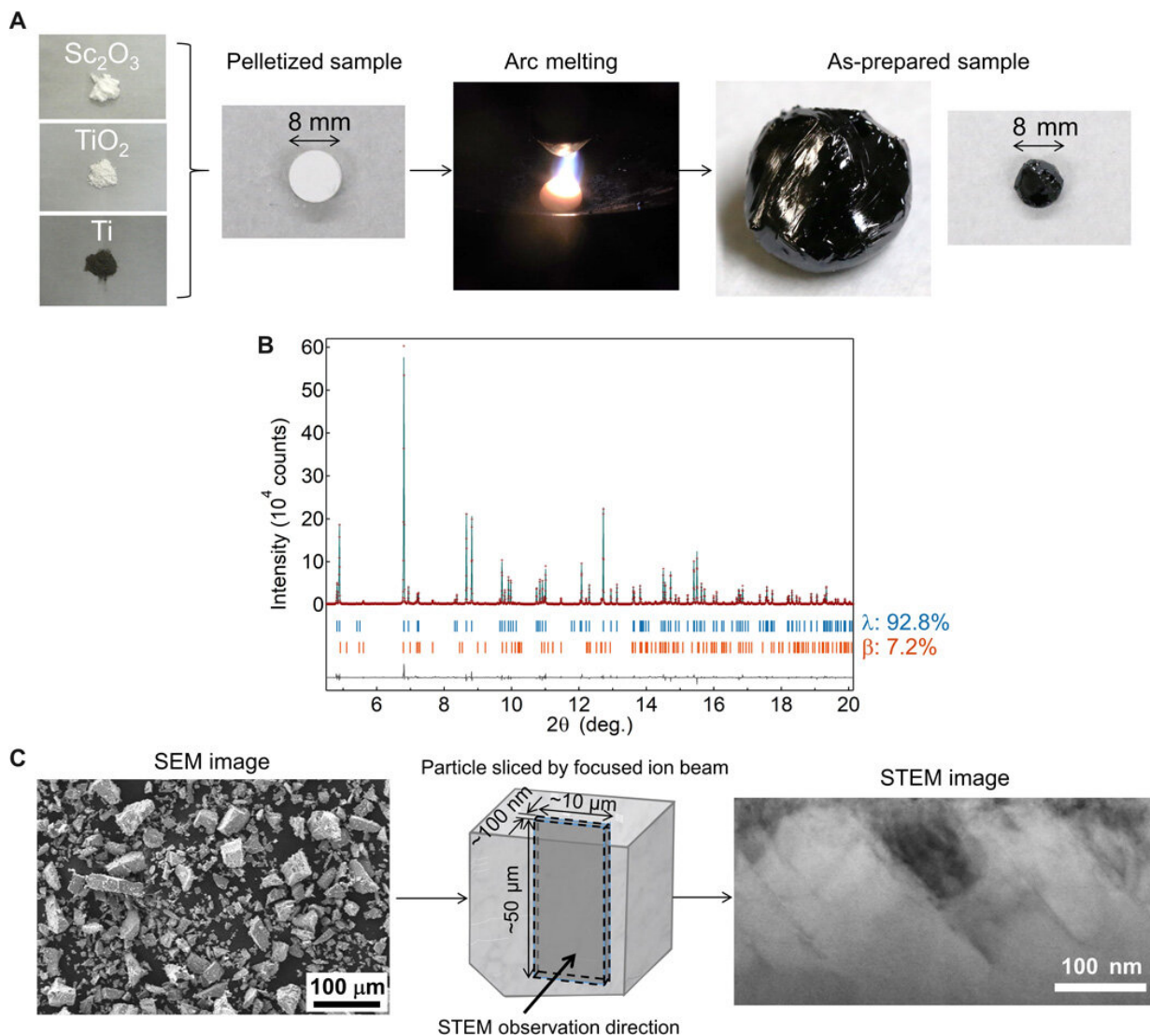
than that of pure λ -Ti₃O₅. Orange elements are those where substituted λ -Ti₃O₅ shows a higher formation energy. (B) Calculated total electronic energies of λ -A_xTi_{3-x}O₅ (A, trivalent elements) and (C) λ -B_xTi_{3-x}O₅ (B, tetravalent elements) in order of atomic number. One of three Ti sites in λ -Ti₃O₅ is substituted by a colored element for the first-principles calculations. Element A in λ -A_xTi_{3-x}O₅ substitutes into the Ti1 site. Element B in λ -B_xTi_{3-x}O₅ substitutes into the Ti2 site. Blue and orange squares represent that elemental substituted λ -Ti₃O₅ shows a lower formation and a higher formation energy, respectively. Black square denotes pure λ -Ti₃O₅. Credit: *Science Advances*, doi: 10.1126/sciadv.aaz5264

Approximately seventy percent of the thermal energy generated in thermal and nuclear power plants is lost as waste heat, with a temperature below the boiling point of water. In a recent report on *Science Advances*, Yoshitaka Nakamura and a research team in chemistry, materials, and technology in Japan developed a long-term heat storage material to absorb heat energy at warm temperatures ranging from 38 degrees C (311 K) to 67 degrees C (340 K). They composed the unique series of materials using scandium-substituted [lambda-trititanium-pentoxide](#) (λ -Sc_xTi_{3-x}O₅). The construct accumulated heat energy from hot water and released the accumulated heat energy upon the application of pressure. The new material has the potential to accumulate the heat energy of hot water generated in nuclear and thermal power plants, then recycle the stored heat energy on demand based on external pressures. The material is also applicable to recycle waste heat in industrial factories and automobiles.

First-principles calculations of formation energy and determining the crystal structure

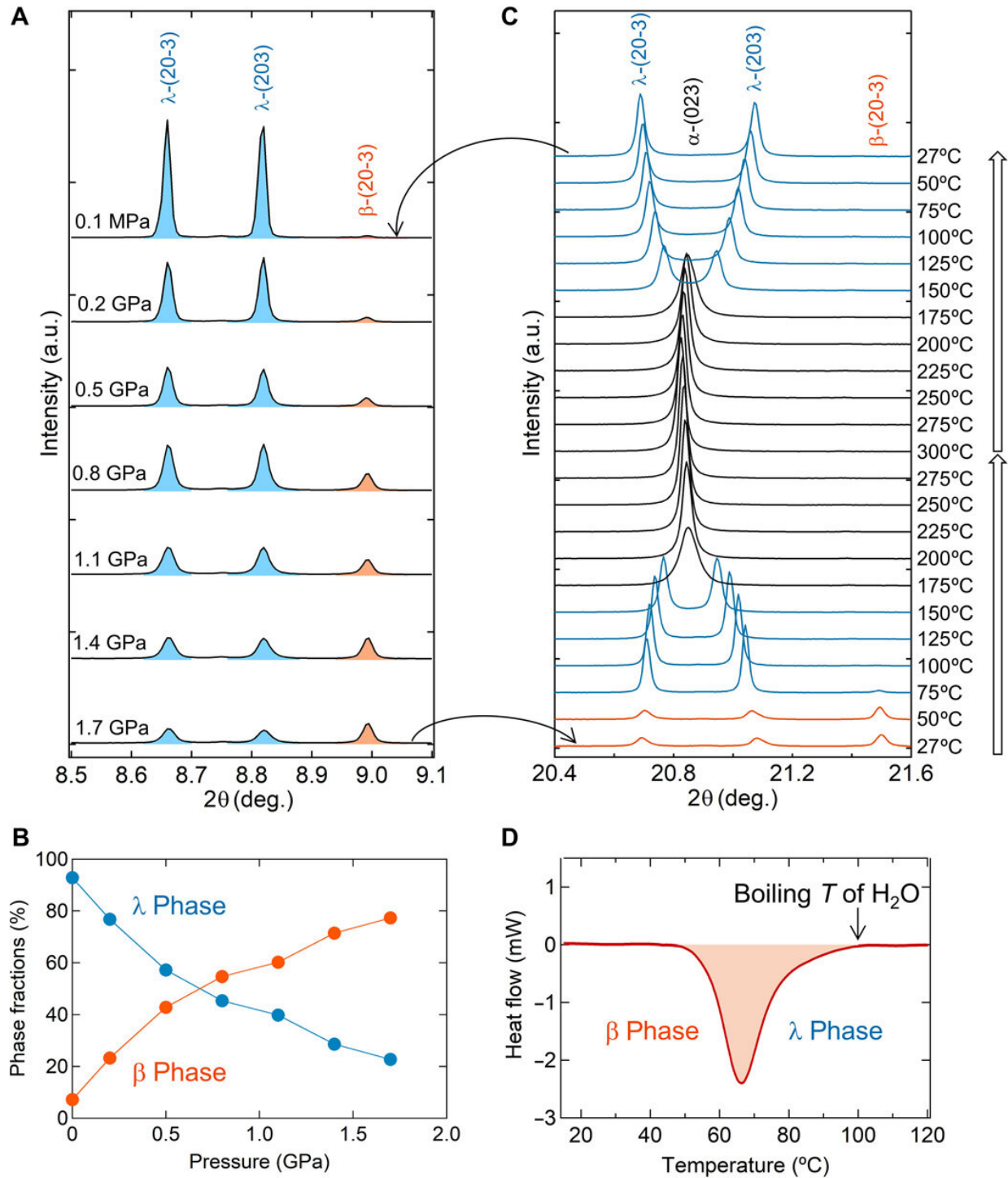
The team used the metal-substituted lambda-trititanium-pentoxide

(λ - $M_x\text{Ti}_3\text{O}_5$) during the experiments to realize heat storage materials that can absorb low-temperature [waste heat](#) and exhibit photo- and pressure-induced [phase transitions](#). Scientists had [previously reported](#) several types of metal-substituted λ - Ti_3O_5 . In this work, Nakamura et al. surveyed 54 elements as metal cations suited for metal substitution of the Ti ion in λ - Ti_3O_5 . Of these, only six had a stabilizing effect including [scandium](#), [niobium](#), [tantalum](#), [zirconium](#), [hafnium](#) and [tungsten](#). The team then reported the synthesis of the crystal structure and heat storage properties of the Sc-substituted λ - Ti_3O_5 in the λ phase.



Synthesis, crystal structure, and morphology of λ -Sc_{0.09}Ti_{2.91}O₅. (A) λ -Sc_{0.09}Ti_{2.91}O₅ sample synthesis. Pelletized mixture powder of Sc₂O₃, TiO₂, and Ti metal with a diameter of 8 mm is prepared, melted, and rapidly cooled in an arc-melting process. After the melting process, the solidified (as-prepared) sample is milled by hand. Photo credit: Yoshitaka Nakamura, Panasonic Corporation. (B) Synchrotron x-ray diffraction (SXR) pattern of the as-prepared Sc_{0.09}Ti_{2.91}O₅ sample collected at room temperature with $\lambda = 0.420111 \text{ \AA}$. Upper blue and lower orange bars represent the calculated positions of the Bragg reflections of λ -Sc_{0.09}Ti_{2.91}O₅ and β -Sc_{0.09}Ti_{2.91}O₅. (C) Scanning electron microscopy (SEM) image of the powdered sample shows a grain size below 100 μm . Particle from the powdered sample is sliced by a focused ion beam. STEM image shows stripe-like domains with a size of about 100 nm \times 200 nm. Scale bars show 100 μm in the SEM image and 100 nm in the STEM image. Credit: *Science Advances*, doi: 10.1126/sciadv.aaz5264

To synthesize the Sc-substituted compound, Nakamura et al. used an arc-melting technique in an Argon atmosphere. During the process, they mixed precursors of Sc₂O₃, TiO₂ and Ti powders to prepare an 8-mm pellet of the mixture shaped into a spherical ball. Then using [X-ray fluorescence](#) (XRF) measurements they determined the formula of the sample (Sc_{0.9}Ti_{2.91}O₅) and performed [synchrotron X-ray diffraction](#) (SXR) to determine the crystal structure. The results corresponded to the crystal structure of λ -Ti₃O₅ with 0.4 percent expansion after metal substitution. Using [scanning transmission electron microscopy](#) (STEM) images the team obtained stripe-like domains in the compound.

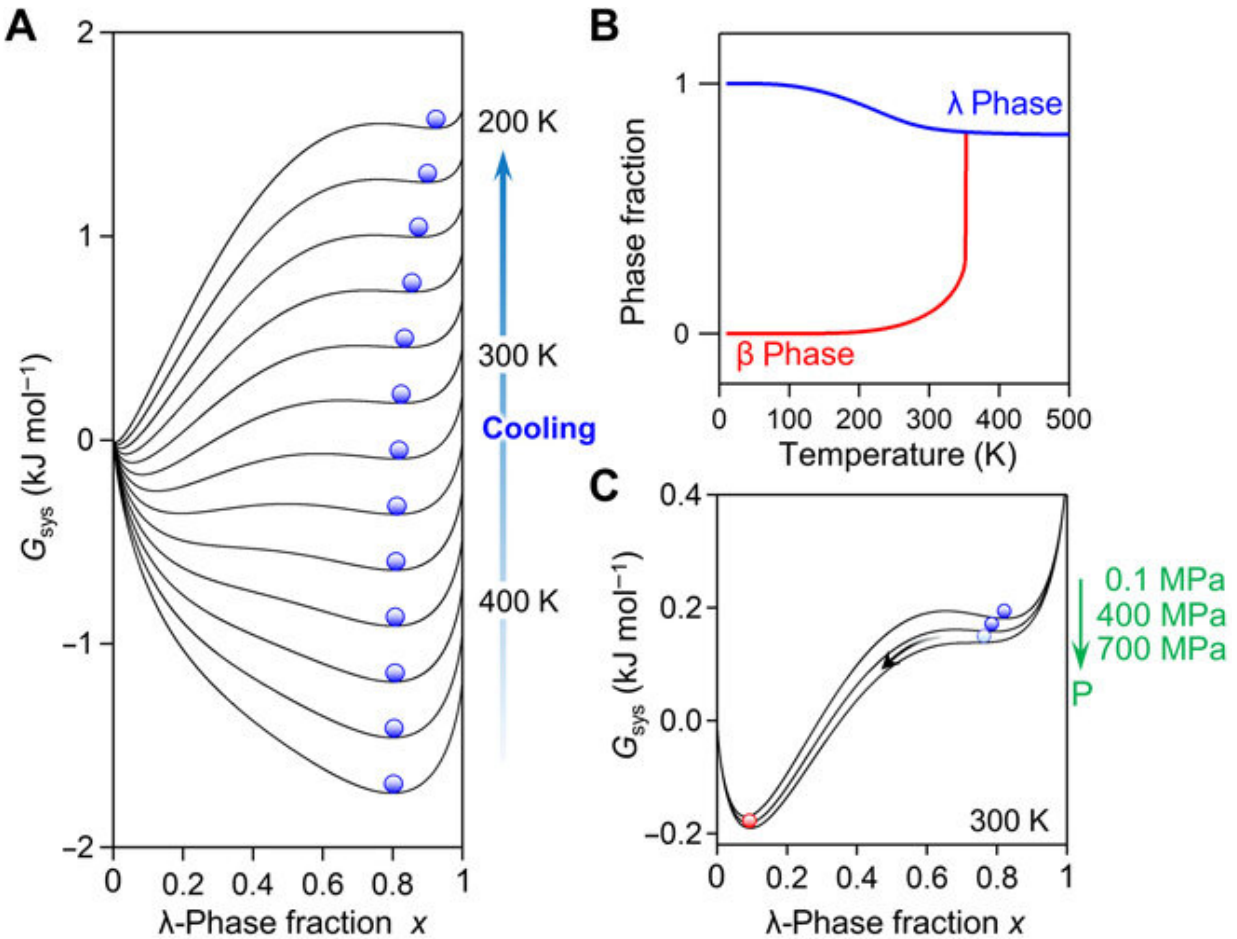


Pressure-induced phase transition and heat-storage process. (A) SXR patterns of $Sc_{0.09}Ti_{2.91}O_5$ measured at room temperature and ambient pressure after compression between 0.2 and 1.7 GPa with a hydraulic press ($\lambda = 0.420111 \text{ \AA}$). As the pressure increases, the λ -(20-3) and λ -(203) peaks (blue) decrease and the

β -(20-3) peak (orange) increases, indicating a pressure-induced phase transition. a.u., arbitrary units. (B) Pressure dependence of the phase fractions of $\text{Sc}_{0.09}\text{Ti}_{2.91}\text{O}_5$ calculated from the SXR D patterns in (A). Crossover pressure (phase transition pressure) occurs at 670 MPa. (C) SXR D patterns of $\text{Sc}_{0.09}\text{Ti}_{2.91}\text{O}_5$ measured between 27°C (300 K) and 300°C (573 K; $\lambda = 0.999255 \text{ \AA}$). The λ and β peaks are constant until 50°C (323 K; orange), and then the β phase decreases and the λ phase increases at 75°C (348 K; blue). The λ phase transforms into the α phase above 175°C (448 K; black) but is restored upon cooling. (D) DSC chart of $\text{Sc}_{0.09}\text{Ti}_{2.91}\text{O}_5$ shows an endothermic reaction at 67°C (340 K). Samples are compressed at 1.7 GPa before the variable temperature SXR D and DSC chart measurements. Credit: *Science Advances*, doi: 10.1126/sciadv.aaz5264

Pressure-induced phase transitions, heat-storage properties, and long-term heat storage mechanisms

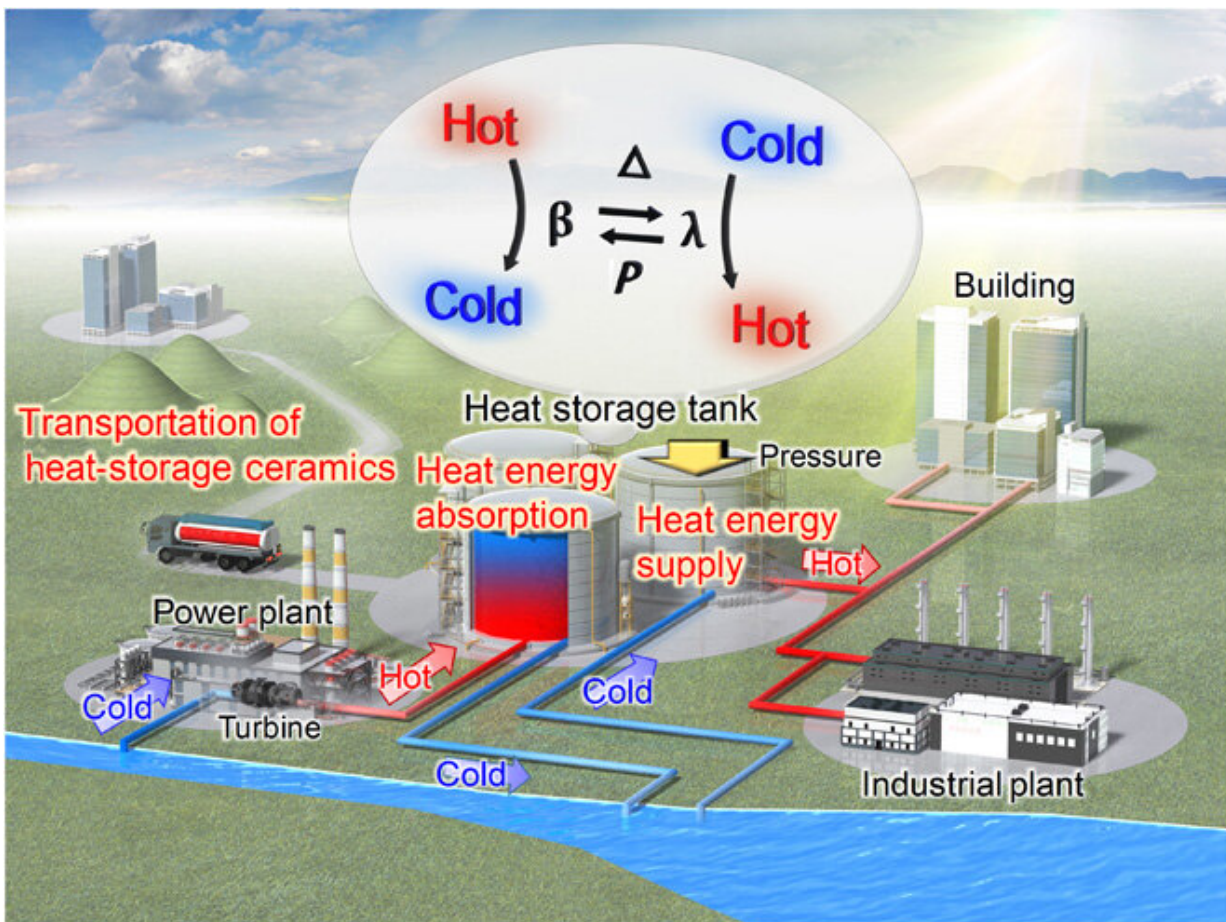
The team next measured the pressure-induced phase transition using SXR D (synchrotron X-ray diffraction) after compressing the samples with a hydraulic press. When the pressure increased, the λ -phase fraction of the sample decreased, and the β -phase fraction increased in a reversible process. They measured the heat absorption mass of the sample after the pressure-induced phase transition (λ - to β -phase) using [differential scanning calorimetry](#) (DSC). They noted the heat absorption of the material with an absorption peak at 67 degrees C and observed repeated pressure- and heat-induced phase transitions. During phase transitions from the β -phase to the λ -phase, the heat storage temperature remarkably reduced from a [previously recorded](#) value of 197 degrees C to 67 degrees C in the present work.



Mechanism of long-term heat storage and pressure-induced phase transition. (A) Gibbs free energy (G_{sys}) versus λ phase fraction (x) curves from 420 to 200 K with a 20 K interval, calculated by the SD model. Blue spheres indicate the thermal population of the λ phase. (B) Temperature dependence of the calculated λ phase (blue) and β phase (red) fractions. (C) G_{sys} versus x under ambient pressures of 0.1, 400, and 700 MPa at 300 K. Credit: *Science Advances*, doi: 10.1126/sciadv.aaz5264

Previous reports on λ - Ti_3O_5 [also credited the reversible phase transition](#) between the λ -phase and β -phase by pressure and heat to the energy barrier between the two phases, which originates from the elastic interaction within the material. To understand the mechanisms of long-

term heat storage and low-pressure induced [heat energy](#) release in this setup, Nakamura et al. calculated the [Gibbs free energy](#) of the system. For this, they used a thermodynamic model based on the [Slichter and Drickamer](#) (SD model). During the process of phase transition, the scientists could maintain the λ -phase for a prolonged time since the energy barrier between the two phases prevented the immediate transfer of the λ -phase in to the β -phase. The resulting $\text{Sc}_{0.9}\text{Ti}_{2.91}\text{O}_5$ prepared in the work showed good stability and could be maintained perfectly for about eight months to one year from the XRD measurement.



Application of Sc-substituted λ - Ti_3O_5 for power plants. Schematic illustration of a heat energy recycling system using Sc-substituted λ - Ti_3O_5 heat-storage ceramics. Cooling water for a turbine in a power plant is pumped from a river or

sea. Water becomes hot after heat exchange through the turbine. This hot water energy is stored in tanks containing Sc-substituted λ -Ti₃O₅ heat-storage ceramics. Water with a reduced heat energy returns to the river or the sea, mitigating the rise of the sea temperature. Energy-stored Sc-substituted λ -Ti₃O₅ heat-storage ceramics can supply heat energy to buildings or industrial plants by applying pressure. Furthermore, the energy-stored ceramics can be transported to distant locations by a truck. Credit: *Science Advances*, doi: 10.1126/sciadv.aaz5264

Proof of concept

The scientists investigated the heat-storage system with Sc-substituted λ -Ti₃O₅ in a practical setting by pumping cooling water for a turbine in a power plant from a river or sea. As the water passed through the turbine, its temperature increased due to heat exchange, transferring the energy of hot water to Sc-substituted λ -Ti₃O₅ materials used in the tanks. Meanwhile, water with a reduced thermal energy returned to the river or the sea. Energy stored in the Sc-substituted λ -Ti₃O₅ could be released in the form of thermal energy by applying pressure for [energy use](#) on demand. Nakamura et al. envision supplying the stored thermal [energy](#) to building or industrial plants that are close to power plants without using electricity.

In this way, Yoshitaka Nakamura and colleagues demonstrated heat storage ceramics based on Sc-substituted λ -Ti₃O₅, which absorbed heat from water. Based on first-principles calculations, they synthesized Sc-substituted λ -Ti₃O₅ ceramics with a heat absorption below 100 degrees C. The heat absorption material recovered [thermal energy](#) from cooling water in power plant turbines and could be easily controlled by changing the Sc content in Ti₃O₅ relative to the application of interest. In addition to its functions in electric power plants, the scientists propose using the materials for heat storage functions by collecting waste [heat](#) from regular

devices such as mobile phones, transport vehicles, from factories and electronic devices.

More information: Yoshitaka Nakamura et al. Long-term heat-storage ceramics absorbing thermal energy from hot water, *Science Advances* (2020). [DOI: 10.1126/sciadv.aaz5264](https://doi.org/10.1126/sciadv.aaz5264)

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