Gwangju Institute of Science and Technology

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Professor Bong-Joong Kim's research team discovers thermal resiliency of organic metal halide perovskite

☐ GIST (Gwangju Institute of Science and Technology, President Kiseon Kim) School of Materials Science and Engineering Professor Bong-Joong Kim's research team succeeded in quantifying the thermal decomposition process of perovskite in high vacuum where oxygen and moisture were removed using a real-time transmission electron microscope * method and formed a single crystal of methylammonium lead iodide perovskite ** nanorod. Through this, it was found that lead iodide *** , which was decomposed at high temperatures, was fully recovered at low temperatures.

* transmission electron microscope (TEM): a microscope that can magnify images over hundreds of thousands of times by transmitting a high voltage electron beam through a thin material

** methylammonium lead iodide perovskite: a solid compound with a perovskite structure having the chemical formula CH3NH3PbX3, (X = I, Br or Cl) and is expected to be used for solar cells, lasers, light emitting diodes, and optical detectors

*** lead iodide (PbI2): at room temperature, it is a bright yellow odorless crystalline solid, that becomes orange and red when heated

☐ Perovskite is a material mainly used in solar cells, and has recently been spotlighted because it shows solar cell power conversion efficiency exceeding 21%. In particular, the single crystal perovskite structure is widely used not only for solar cells but also for X-ray detectors, gamma-ray detectors, and visible light detectors due to absorption, faster charge transfer, and high stability that shift to the red wavelength band.

- To make a solar cell with high light conversion efficiency, high quality crystallinity and morphology * are required. To this end, an intermediate phase ** is produced using a antisolvent engineering method *** and heated to produce crystalline perovskite. However, the temperature given for these phase changes is too high or the increasing temperature in the operation of solar cells, which breaks down perovskite to remove iodide lead, and continues to remain even after the battery has stopped working, resulting in a rapid reduction in battery efficiency.

  * morphology: form or shape of a substance

  ** intermediate phase: thermodynamically quasi-stable phase

  *** antisolvent engineering: a technique for extracting solids from a solution

☐ In this study, the first single crystal intermediate phase nanorods were synthesized using the antisolvent engineering method and heated in a high-vacuum environment where oxygen and moisture were controlled to control the crystal structure and crystal orientation of the intermediate phase, perovskite, and precipitated lead iodide. Furthermore, the volume of lead iodide particles was measured according to temperature by giving a temperature cycle up to 155 degrees Celsius, thereby obtaining the enthalpy * for decomposing perovskite into lead iodide. It was also found that during the precipitation of lead iodide, the methylammonium lead iodide molecule did not evaporate and was over-concentrated in the perovskite, creating a new form of thermodynamic state.

  * enthalpy: one of the physical quantities used in thermodynamics where the amount of pressure applied outside the system and the volume multiplied by it, adding to the internal energy of the system

- Surprisingly, it was confirmed that lead iodide precipitated at high temperature recovered to single crystal perovskite at low temperature, and carrier mobility *, trap density **, and dielectric constant *** were also restored.

  * carrier mobility: defined by the ratio of the electron's drift velocity to the electric field applied from the outside

  ** trap density: defect density in a substance that limits the movement of charges

  *** dielectric constant: when an electric field is applied between electric charges, a physical unit representing the effect of the medium between the electric charges on the electric field

☐ Professor Bong-Joong Kim said, "The results of this study not only presented a fundamental solution to the study of perovskite solar cells that are at the limit of weak thermal stability and increased efficiency, but was also the first case of quantitatively identifying the thermodynamic properties of organic metal halide perovskite."

☐ This research was led by GIST School of Materials Science and Engineering Professor Bong-Joong Kim (corresponding author), conducted by researcher Yong-Ryun Jo (first author), supported by Samsung Research Funding Center of Samsung Electronics, and was published on May 7, 2020, by *ACS Central Science* (IF: 12.837), a renowned international journal in the field of material chemistry. It was also selected as the cover paper for the journal because its importance was widely recognized by academics and the general public.

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