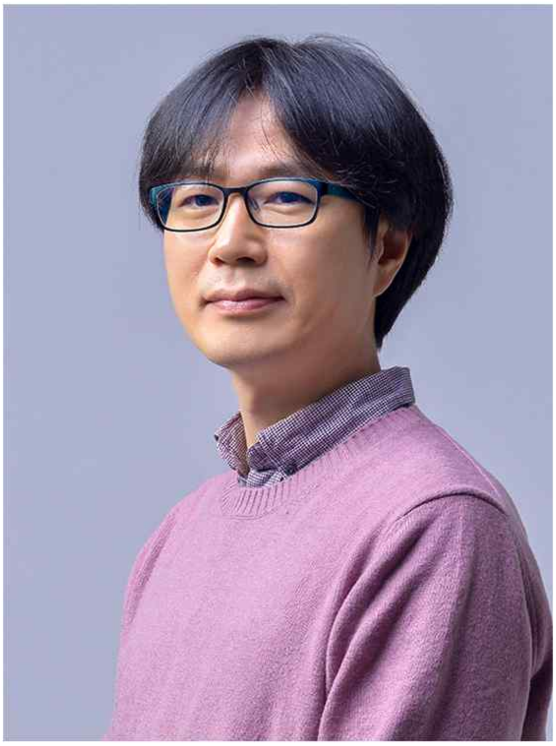
GIST and Sogang University joint research team unravel the principle of structural change in high-pressure phase matter: Step-by-step structural transitions of two-dimensional Weyl semimetals and the link between superconductivity and the phenomenon are experimentally proven

- Professor Jong Seok Lee's team in the Department of Physics and Photon Science quantitatively elucidates the interlayer and intralayer structural changes of van der Waals Weyl semimetals in a high-pressure environment, and experimentally proves the close relationship between structural transition and superconductivity

- Presents a step-by-step structural transition model, establishing an important theoretical foundation for high-pressure property research and the development of next-generation quantum materials such as spintronics and quantum computing… Published in the international academic journal 《NPG Asia Materials》



▲ (From left) Professor Jong Seok Lee and Dr. Hwiin Ju of the Department of Physics and Photon Science

The Gwangju Institute of Science and Technology (GIST, President Kichul Lim) announced that the research team of Professor Jong Seok Lee of the Department of Physics and Photon Science, in collaboration with Sogang University, has clarified how two-dimensional materials (WTe_2, $MoTe_2$) known as 'van der Waals Weyl semimetals*' change their structure and electronic properties in a high-pressure environment.

This study is drawing attention as it experimentally proves that the structural transition of topological materials and the phenomenon of superconductivity* are closely linked under high-pressure conditions.

* Van der Waals Weyl semimetal: A special two-dimensional metal material in which atomic layers are loosely bound by van der Waals forces, and electrons exhibit a unique quantum property called the 'Weyl state'. Representative examples include WTe_2 (tungsten ditelluride) and $MoTe_2$ (molybdenum ditelluride), which exhibit unique phenomena such as the unusual Hall effect, giant magnetoresistance, and Fermi arc due to their asymmetrical structure and strong spin-orbit coupling. In particular, $MoTe_2$ can switch between topological metals and superconductors depending on the temperature, and is attracting attention in the fields of next-generation electronic devices and quantum technology.

* Superconductivity: A physical phenomenon in which a specific material completely loses electrical resistance and blocks external magnetic fields (Meissner effect) at extremely low temperatures (critical temperature). In this state, current can flow permanently without energy loss, and magnetic levitation, in which a magnet floats in the air, is also observed.

The superconductivity phenomenon is applied to cutting-edge technologies such as power transmission without power loss, high-magnetic field devices (MRI), magnetic levitation trains, and quantum computers, and the development of superconductors that operate at room temperature and pressure is currently receiving attention as a key task.

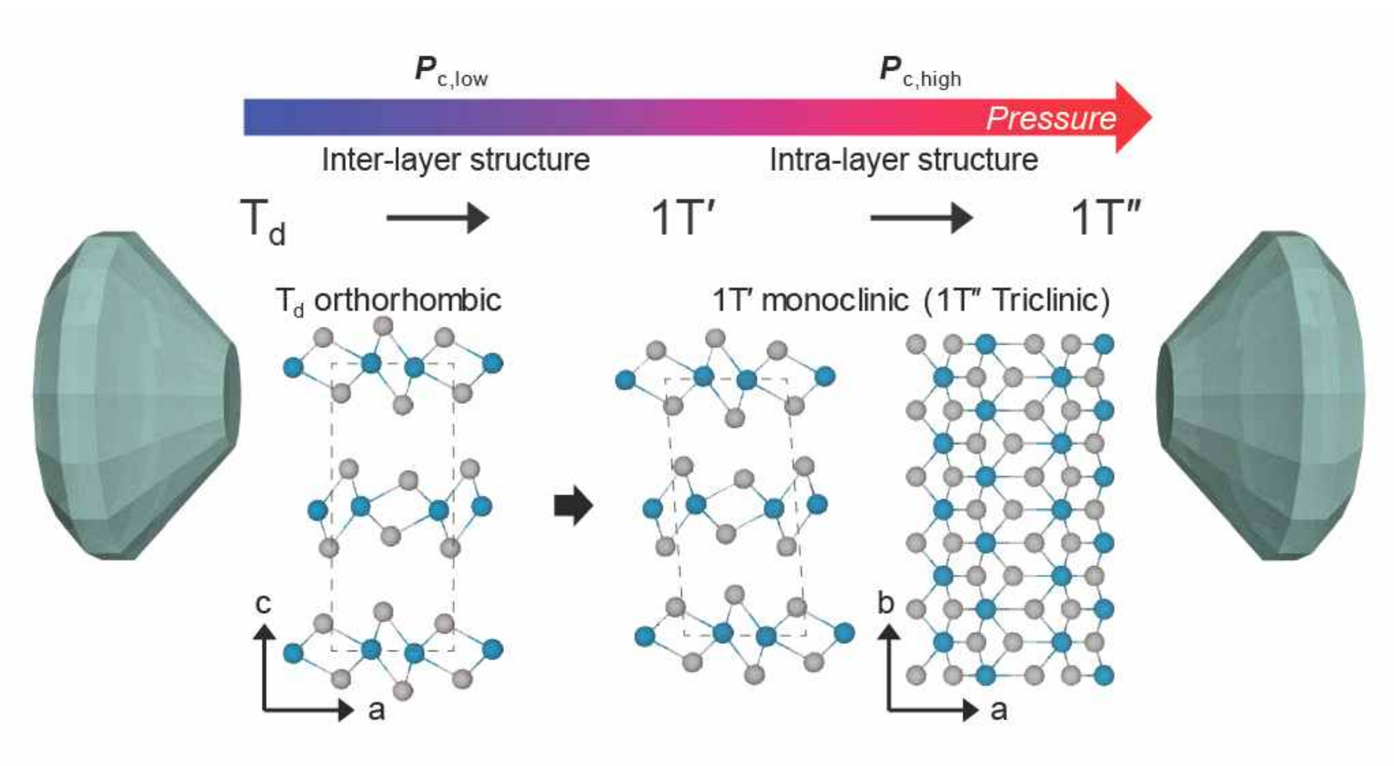
In particular, the research team quantitatively proved that the structure of van der Waals materials changes differently between layers (inter-layer) and within layers (intra-layer) when pressure is applied, and suggested a new structural change model that can explain this, thereby increasing academic value.

The results of this study are expected to be utilized as an important theoretical basis for the development of nano and quantum materials as well as high-pressure material research.

Van der Waals materials have a structure in which thin atomic layers are stacked one after another, and the bonding between each layer is very weak, so they have the characteristics of a two-dimensional material and strong directionality (anisotropy).

When the Weyl semimetal properties are added here, 'Weyl fermions' that behave like massless particles when current flows appear, which is also a very interesting subject from a physical perspective.

The core of this study is that the structure of van der Waals Weyl semimetals (WTe_2, $MoTe_2$) changes stepwise depending on pressure, and this structural transition is directly connected to the change in electronic state and the onset of superconductivity.



▲ Summary of structural changes in WTe_2 according to pressure. When applying pressure of several gigapascals through a diamond anvil cell, the crystal structure changes sequentially from the Td (tetragonal) structure to the 1T′ (monoclinic) structure, and then to the 1T′′ (triclinic) structure.

In particular, it was confirmed that at a pressure of approximately 2.5 gigapascals (GPa), a structural transition occurred in WTe_2 from the Td (tetragonal) structure to the 1T′ (monoclinic) structure, and that the magnetoresistance decreased rapidly and superconductivity appeared simultaneously.

These results were clearly observed through Raman spectroscopy* and optical pump-probe spectroscopy* measurements, proving a direct link between structural transitions and changes in electronic properties and the onset of superconductivity.

* Raman spectroscopy: A non-contact, non-destructive analysis technique that investigates low-energy modes such as vibrations and rotations in molecules or solids. Based on the inelastic scattering phenomenon discovered by Indian physicist C.V. Raman, it analyzes the wavelength change (Raman scattering) that occurs when laser light of a specific wavelength interacts with a sample to obtain information such as molecular structure, bonding state, crystallinity, and stress. It is possible to analyze various samples such as liquids, solids, and gels without separate preprocessing, and is used in various fields such as semiconductors, bio, energy materials, and art appraisal.

* Optical pump-probe spectroscopy: A dynamic spectroscopy technique that uses ultra-fast laser pulses in the femtosecond (fs) unit to track the energy state or structural changes of a material in real time over time. First, the sample is stimulated with a 'pump' pulse, and then the response is measured with a 'probe' pulse after a certain period of time to observe ultrafast phenomena such as electronic transitions, vibrational relaxation, and structural changes. This technology is used to elucidate chemical reaction mechanisms, analyze semiconductor charge transfer, and analyze changes in biomolecular structure, and is considered a key tool in ultrafast spectroscopy and femtochemistry research.

Another important discovery is that the structural transition occurs in two stages as the pressure increases.

At low pressures, the interlayer structure changes first, and then, at high pressures of about 10 GPa or more, the atomic arrangement within the layer becomes distorted and transitions from the 1T′ (monoclinic) structure to the 1T′′ (triclinic) structure.

This high-pressure transition was experimentally proven by the rapid change in the second harmonic (SHG) signal, the disappearance of the Raman mode, and the change in optical reflectivity, and it coincides exactly with the previously known change in charge concentration, providing important clues to elucidating the complex multi-step mechanism of structural transition in a high-pressure environment.

Professor Jong Seok Lee said, "This study is meaningful in that it experimentally confirms the connection between structural transition, phase state change, and onset of superconductivity, and presents a model for structural change according to pressure, thereby establishing a new theoretical foundation for high-pressure research." He explained, "It will serve as an important starting point for the development of phase control technology in spintronics and quantum computing devices in the future by revealing that the structure and electronic properties are closely linked in two-dimensional topological materials."

This study, supervised by Professor Jong Seok Lee of GIST and conducted by Dr. Hwiin Ju, involved researchers from Seoul National University, Sogang University, Korea Research Institute of Standards and Science, and POSTECH, and was supported by the Ministry of Science and ICT and the National Research Foundation of Korea's Mid-career Researcher Support Program. The research results were published online in the international academic journal 《NPG Asia Materials》 on April 30, 2025.

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