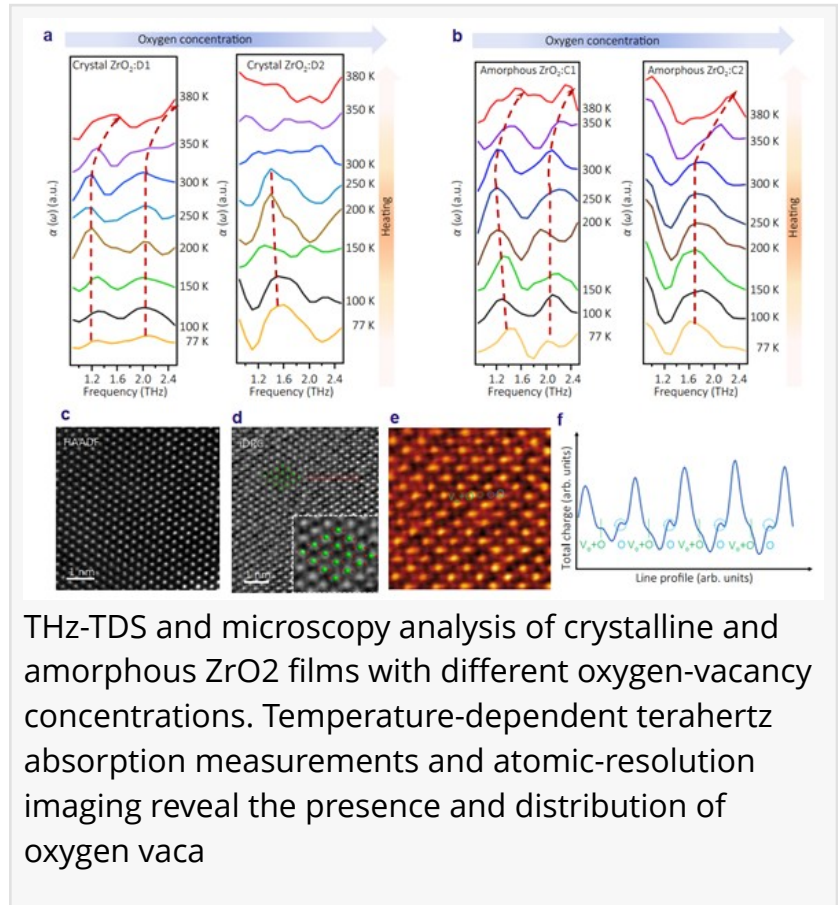


Vacancy Oscillating Mode in Amorphous Binary Oxide Film by Terahertz Time Domain Spectroscopy

THz-TDS demonstrates oxygen-vacancy oscillation modes underlying ferroelectric-like behavior in amorphous zirconia films

CHINA, July 13, 2026 /

EINPresswire.com/ -- Terahertz time-domain spectroscopy (THz-TDS) provides new insights into oxygen vacancy oscillation modes in amorphous zirconia films. Researchers from Xidian University, the Beijing Academy of Quantum Information Sciences, and Huazhong University of Science and Technology used THz-TDS along with infrared spectroscopy and first-principles calculations to demonstrate that oxygen-vacancy migration play a key role in ionic conductivity and ferroelectric-like behavior



With the rapid development of emerging information technologies such as big data, cloud computing, and artificial intelligence, the demand for massive data storage and processing has placed increasingly stringent requirements on memory devices. Novel nonvolatile memories are regarded as a key foundation for future memory-computing architectures. Among them, ferroelectric random-access memory (FeRAM) and resistive random-access memory (RRAM) have attracted significant attention owing to their low power consumption and excellent compatibility with complementary metal-oxide-semiconductor (CMOS) technology. Binary oxides represented by hafnium oxide (HfO₂) and zirconium oxide (ZrO₂) are not only widely used as high-k gate dielectrics in the modern semiconductor industry, but have also emerged as promising materials due to their controllable ferroelectric and resistive-switching properties.

Meanwhile, as technology scaling approaches and surpasses the 5 nm node, a growing number of studies have revealed pronounced ferroelectric-like behavior even in amorphous binary oxide films with thicknesses down to approximately 1 nm. Our previous research indicated that the reversible motion of oxygen ions is the most critical factor involving ferroelectric behavior in these amorphous or polycrystalline binary oxide films. Therefore, understanding the distribution and dynamic behavior of oxygen vacancies is essential for elucidating the physical mechanism underlying ferroelectric-like phenomena in amorphous oxides. However, due to the lack of long-range structural order in amorphous materials, oxygen vacancies are difficult to directly observe using conventional structural characterization techniques, and their microscopic role during polarization switching remains largely elusive.

Terahertz time-domain spectroscopy (THz-TDS) offers a promising approach to address this challenge. The energy scale of terahertz radiation, ranging from a few to several tens of millielectronvolts, closely matches that of ion hopping, localized vibrations, and defect-related low-energy excitations. By probing the absorption and transmission of terahertz waves through materials, THz-TDS can indirectly detect localized states and ionic oscillation modes associated with oxygen vacancies, thereby providing microscopic migration-energy information that is inaccessible to conventional low-frequency impedance spectroscopy. Motivated by this opportunity, a collaborative research team from Xidian University, the Beijing Academy of Quantum Information Sciences, and Huazhong University of Science and Technology employed THz-TDS to directly probe vacancy oscillation modes in amorphous oxide films, aiming to reveal the intrinsic relationship between oxygen-vacancy migration and polarization behavior.

The research team employed THz-TDS to reveal the vacancy oscillation mode in amorphous ZrO_2 films and investigate its critical role in ionic conductivity. By combining THz-TDS, infrared reflectivity measurements, and first-principles density functional theory (DFT) calculations, the researchers systematically studied the optical absorption and reflection characteristics of both crystalline and amorphous ZrO_2 thin films with different oxygen-vacancy concentrations. Their work was published in Volume 9, Issue 6 of [Opto-Electronic Advances](#) on June 07, 2026.

Experimental results show that oxygen vacancy migration rather than the intrinsic paraelectric nature in films significantly affects the conductivity and polarization behavior of ZrO_2 thin film. Notably, except for the phonon modes that induce distinct absorption peaks around 11 THz, additional absorption peaks are observed in the 1–2 THz range, which are caused by localized states originated from the oxygen vacancies, supported by DFT calculations. Temperature-dependent ion migration behavior further confirms the role of vacancy oscillation modes in ionic conductivity. DFT calculations additionally reveal how oxygen vacancies alter infrared absorption and optical modes, leading to a redshift in existing absorption peaks or the introduction of new peaks. These findings establish a more comprehensive physical framework for understanding ferroelectric-like phenomena in amorphous oxide materials and enriching the fundamental theory of amorphous ferroelectric systems.

From an application perspective, this work provides a new technological pathway toward next-generation ultra-low-power nonvolatile memories. Since amorphous binary oxides can be

directly fabricated by low-temperature atomic layer deposition (ALD) without requiring conventional high-temperature crystallization processes, they offer excellent CMOS compatibility and strong potential for back-end-of-line (BEOL) integration. This strategy may help overcome key challenges associated with advanced technology nodes, including equivalent oxide thickness (EOT) scaling and thermal-budget limitations, thereby enabling new material platforms for future high-density memories, neuromorphic computing hardware, and in-memory computing systems.

Looking forward, further efforts will focus on optimizing THz characterization techniques to enable in-situ and operando observations under multiple external stimuli, such as electric fields and mechanical stress. Future studies will also aim to establish precise control over oxygen-vacancy concentration and distribution, while exploring new oxide ferroelectric-like materials with enhanced performance and functionality.

Reference

Title of original paper: Vacancy oscillating mode in amorphous binary oxide film by terahertz time domain spectroscopy

Journal: Opto-Electronic Advances

DOI: <http://doi.org/10.29026/oea.2026.250217>

About Haiyun Liu from the Beijing Academy of Quantum Information Sciences

Haiyun Liu is an Associate Researcher in the Ultrafast Spectroscopy Group at the Beijing Academy of Quantum Information Sciences. As a corresponding author, he has published 13 SCI papers in leading journals, including Physical Review Letters, Nano Letters, Optics Express, and InfoMat. His group is dedicated to quantum state studies using a full-spectrum ultrafast spectroscopy platform spanning the visible–infrared–terahertz range. His research focuses on carrier dynamics, light–matter interactions in strong and weak coupling regimes, ultrafast optical control of quantum materials, and ultrafast optoelectronic devices. His main interests include exciton–polariton lasing and room-temperature Bose–Einstein condensation.

About Kanhao Xue from Huazhong University of Science and Technology

Kanhao Xue is a professor at the School of Integrated Circuits, Huazhong University of Science and Technology. He has authored more than 170 papers in international journals, such as Physical Review Letters. He has led multiple research projects, including National Key Research and Development Project, National Natural Science Foundation of China projects, and industry collaborations with Huawei and Gaode Infrared. He has been recognized as a Highly Cited Researcher in Elsevier's global top 2% scientists list. His research focuses on semiconductor band-structure calculation methods and hafnium-oxide-based nanoelectronic devices. He proposed the shell DFT-1/2 method and the seven-coordination theory for hafnia-based ferroelectricity.

About Yan Liu from Xidian University

Yan Liu is a professor at the School of Microelectronics, Xidian University. She has long been engaged in research on novel semiconductor functional devices, with pioneering contributions to

micro/nano photonic devices, post-Moore electronic devices, and optoelectronic integration. She currently leads multiple major research projects supported by the National Natural Science Foundation of China and the National Key Research and Development Project. She has published more than 150 papers in leading journals and conferences, including IEDM, IEEE Electron Device Letters, Optics Express, and Laser & Photonics Reviews, and has delivered more than 10 invited talks at international conferences.

Funding information

The authors received support from the National Key Research and Development Project (Grant Number: 2023YFB4402303), the National Natural Science Foundation of China (Grant Numbers: 62204226, 62374151, 62574159, 62025402, 62090033 and 92264202), Major Program of Zhejiang Natural Science Foundation (Grant Number: DT23F0402).

Siyi Ma

Institute of Optics and Electronics, Chinese Academy of Science

+ 19136186296

[email us here](#)

This press release can be viewed online at: <https://www.einpresswire.com/article/926196446>

EIN Presswire's priority is source transparency. We do not allow opaque clients, and our editors try to be careful about weeding out false and misleading content. As a user, if you see something we have missed, please do bring it to our attention. Your help is welcome. EIN Presswire, Everyone's Internet News Presswire™, tries to define some of the boundaries that are reasonable in today's world. Please see our Editorial Guidelines for more information.

© 1995-2026 Newsmatics Inc. All Right Reserved.