22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

Direct Observation of Atomic Diffusion at Grain Boundaries in Oxides

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Grain Grain boundaries and interfaces play a central role in determining the macroscopic properties of ceramic materials. This is because their atomic structure and local chemistry are easily altered by the segregation of dopants and impurities, as well as by mass transport along interfaces. Recent developments in aberration-corrected scanning transmission electron microscopy (STEM), particularly when combined with in situ observation and first-principles calculations, now allow these interfacial processes to be examined quantitatively at the atomic scale. In this presentation, grain boundaries are described not as fixed structural defects, but as metastable systems that respond sensitively to changes in chemical composition and external driving forces. Under such conditions, they can undergo structural transformations. These transformations are closely related to important kinetic processes—grain-boundary migration and diffusion—that control microstructural evolution during ceramic processing. Studies of doped alumina provide clear examples of these effects. They show that grain-boundary migration strongly depends on grain boundary character, and that solute segregation can induce grain-boundary phase transformations. Such transformations can significantly change diffusion behavior and may even lead to positive feedback between chemical segregation, structural change, and transport. By combining atomic-resolution experiments with computational and data-driven approaches, this work clarifies key mechanisms governing grain-boundary behavior and offers practical guidelines for designing advanced ceramic materials through microstructure control.

[1] J. Wei, B. Feng, R. Ishikawa, T. Yokoi, K. Matsunaga, N. Shibata and Y. Ikuhara: Nat. Mater., 20, 951–955 (2021).
[2] C. Yang, B. Feng, T. Futazuka, N. Shibata and Y. Ikuhara: Nat. Commun., 16, 9707 (2025).
[3] T. Futazuka, R. Ishikawa, T. Yokoi, K. Matsunaga, N. Shibata and Y. Ikuhara: Nat. Commun., 16, 9043 (2025).