23rd International Conference on
Diffusion in Solids and Liquids
20 TO 24 JUNE 2027 | PARIS, FRANCE

ABSTRACT:

Atomistic Modelling of Carbon Ordering and Decomposition in BCC Fe: Formation of Metastable Carbides

Iron–carbon materials have played a major role in human history, from early iron production and ancient steelmaking to the development of modern structural materials. Iron carbides have also been identified in historical steel materials, including Damascus steel, whose remarkable mechanical properties have inspired extensive investigations into the relationships between microstructure and performance. Today, iron carbides are attracting renewed interest not only in metallurgy but also as nanostructured materials with potential applications in magnetic technologies, catalysis, and biomedical imaging. Understanding how these phases form and how their structures and properties can be controlled therefore remains relevant to both fundamental science and materials engineering. This lecture will present atomistic modelling results on carbide formation during martensite ageing using the atomic density function (ADF) method. Particular attention will be paid to the kinetics of carbon redistribution and ordering on the octahedral interstitial sublattices of body-centred cubic (BCC) iron. Building on the theoretical framework developed by Khachaturyan, carbide formation is investigated as a sequence of coupled decomposition and ordering transformations driven by elastic interactions and structural relaxation. The modelling provides insight not only into the atomic arrangements and crystal structures of individual metastable carbides, but also into the kinetic pathways connecting them, revealing the intermediate configurations and successive transformations involved in their formation. These results contribute to a deeper understanding of the mechanisms governing Fe–C microstructure evolution during ageing and tempering.