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X-ray tracing for the analysis of microstructures during the alpha–epsilon transition in iron under pressure

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Abstract

Phase transitions in metals have a considerable influence on their mechanical response and therefore are of fundamental importance to industry. Some of these transitions are classified as martensitic, a transformation mechanism involving small (but collective) atomic displacements that give rise to characteristic microstructures. The microstructures formed in single-crystal iron under loading are complex, as they are composed of the six deformation variants of the high-pressure phase [1]. Post-mortem analyses of iron single crystals subjected to short laser-driven shock loadings (duration < 20 ns) reveal extremely elongated reversion structures, in apparent contradiction with the short loading times, and suggesting the possible formation of similarly extended microstructures under pressure [2]. To better understand this discrepancy between the spatial extent of the microstructures and the high kinetics of the transformation, we aim to develop links between full-field simulations (the “Phase-Field by Reaction Pathway,” PF-RP, [3–5]) and X-ray diffraction patterns, such as those obtained at state-of-the-art synchrotron facilities. We will present a numerical simulation methodology for microstructure formation in pure iron, combining PF-RP with multiphase crystal plasticity [5], and discuss the role of plasticity in microstructure development under high pressure. The relevance of these results will be assessed through comparison with high-pressure X-ray tomography measurements [6], which are in situ and non-destructive techniques that have made it possible to track the successive stages of the transformations and clarify their fundamental mechanisms.

The method used to generate simulated X-ray diffraction spectra (X-ray tracing method) will then be presented and compared with experiments conducted in diamond anvil cells [1]. The various possible artifacts will be discussed.

Keywords:

XRay tracing martensite iron phase transition

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