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Microstructures induced by phase transformations under extreme conditions

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Phase transitions in metals have a drastic influence on their mechanical response and thus have a fundamental bearing for the industry. Some of them are described as martensitic, a displacive mechanism involving small but collective atomic displacements which induces characteristic microstructures. Metals also exhibit a rich polymorphism under extreme conditions (high pressure – high temperature), but the mechanism of transitions were unknown as the microstructures formed could not be measured with conventional techniques such as powder X-ray diffraction.

We characterized pressure-induced phase transformations in iron (alpha-epsilon) and cerium (gamma-alpha), pressurizing samples in diamond anvil cells or Paris-Edinburg presses in the 0-20 GPa, 300-100 K pressure-temperature range. The use of samples with controlled microstructures, together with in situ measurements – single and multigrain X-ray diffraction, X-ray computed tomography coupled with diffraction – allows constraining their mechanisms and observing transient states. The in situ observables are transformation conditions, elastic strains, orientation relations, surfaces of coexistence between the two phases. They are complemented by ex situ scanning electron microscope analysis (EBSD technique) and interpreted using mechanical modelling.

For iron, we find that the first displacive step along Burgers path (see Figure) can be followed by a reconstructive stage, the microstructure keeping a memory of the first step. This memory triggers the reverse transformation path. Transformation twinning affects a limited volume of the sample. For cerium, the transformation microstructure exhibits martensitic features, such as platelets, which could be explained by an elastic softening in gamma-Ce. Such monitoring of allotropic transitions can be used to tailor materials with outstanding mechanical or thermal properties.

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epsilon-Fe platelets orientation variants predicted

