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In situ X-ray diffraction study of niobium under extremely high hydrostatic pressures

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Niobium is widely used as an alloying element for the steelmaking industry, high-temperature materials for the aerospace industry, and in Li-ion batteries. However, the knowledge of niobium's phase diagram is still limited, and there are few studies on this subject. In such a context, understanding how niobium behaves under high hydrostatic pressures is a fundamental step towards advancing knowledge of the phase transformations that can occur in these conditions. Here, niobium powder was subjected to 0.8, 6.5, and 10 gigapascals using a Diamond Anvil Cell with He as a hydrostatic medium. At these pressures, two-dimensional X-ray diffraction patterns were acquired at the synchrotron Extreme condition Methods of Analysis beamline. The X-ray data was integrated using GSAS-II software, and the obtained one-dimensional patterns were analyzed using the Rietveld method. The profile parameters were post-processed following the Williamson-Hall methodology to determine coherently scattering domain size and crystallite defect density. Here, it was found that when pressure increased from 0.8 GPa to 10 GPa, the lattice parameter decreased from 3.308 Å to 3.259 Å. This change occurred simultaneously with an increase of 0.5E13 m-2 in crystallographic defect density. Our results suggest that microstructural inhomogeneities induce plastic deformation in the sub-grain structures.