

**Supplementary materials for**  
**Anisotropic Thermoelastic Properties of Fe<sub>7</sub>C<sub>3</sub> at High Pressures by Single-Crystal**  
**X-Ray Diffraction**

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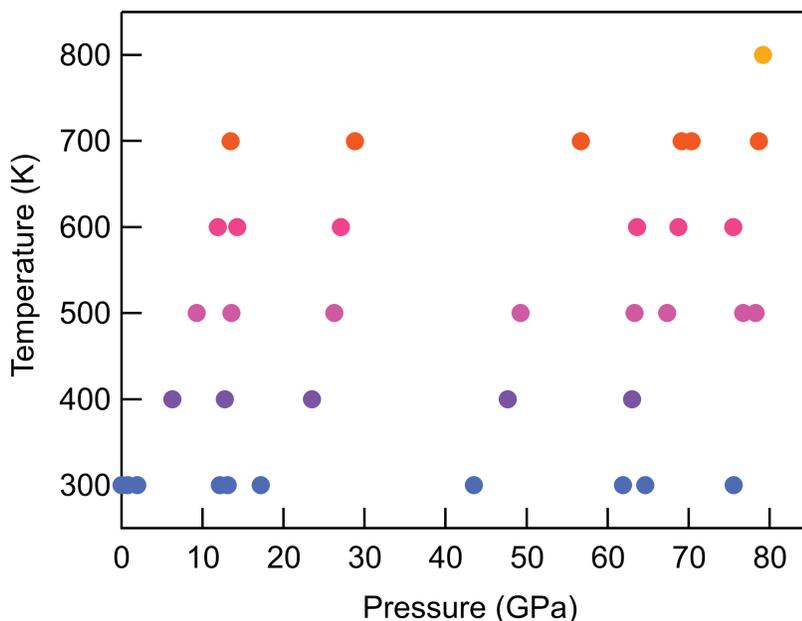


Figure S1. The *P-T* coverage of the XRD experiments of Fe<sub>7</sub>C<sub>3</sub> in the diamond anvil cell.

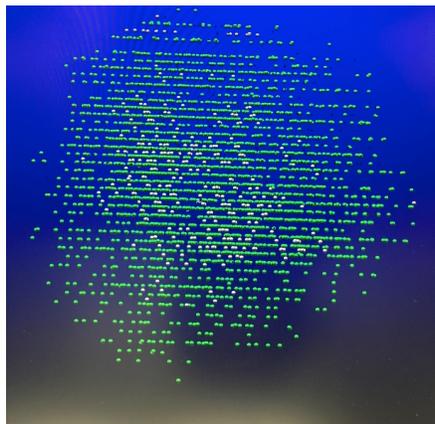


Figure S2. All the peaks harvested from single-crystal XRD measurements of  $\text{Fe}_7\text{C}_3$  at UHM. The green peaks were used for indexing and refinement of the crystal structure at ambient conditions and may correspond to a dominant twin domain (as described in the main text). The white peaks are unique to the secondary twin domain. This corresponds to a  $180^\circ$  rotation around the  $[-1\ 0\ 2]$  axis.

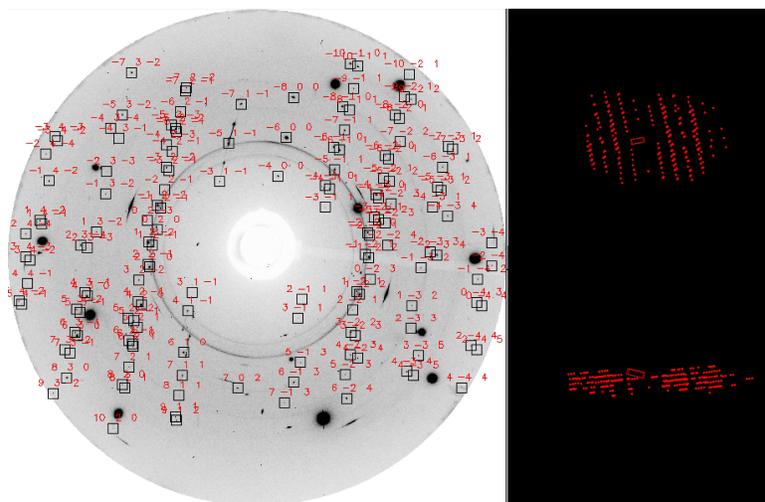


Figure S3. The representative single crystal XRD image at 28.8 GPa and 700 K(left) and projections of the  $\text{Fe}_7\text{C}_3$  crystal structure in reciprocal space along different crystallographic directions (right). Red labels in the measured patterns correspond to Miller indices (hkl) of the reflections. The upper right projection is perpendicular to the X-ray beam.