PRESSURE-INDUCED STACKING DISORDER AND TRIGONAL DISTORTION IN $PbFe_{12}O_{19}$ HEXAFERRITE

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High-pressure X-ray diffraction (XRD) experiments on $PbFe_{12}O_{19}$ (M-type lead hexaferrite, ambient $P6_3/mmc$ structure) reveal a structural distortion between 8 and 25 GPa, manifesting as stacking disorder along the c-axis and trigonal symmetry breaking. At ambient conditions and up to ~29 GPa, prior studies report isostructural compression with no phase changes [1].

Here, using diamond anvil cell (DAC) XRD (Cu Kα), a new low-angle peak emerges at 4.8° 2θ (d ≈ 18.38 Å) at 8 GPa, alongside activation of the forbidden (003) reflection (*l*=3 odd, absent in $P6_3/mmc$). Rietveld refinement (FullProf) of the 8 GPa pattern requires a 1×1×3 supercell (c ≈ 68 Å, multiplicity m=3) with reduced P31m symmetry (157), yielding low $R_{wp} \approx$ 5–8% and indexing all peaks, including (004) for the new reflection and (003) via trigonal allowance (00l: l=3n).

This distortion arises from extreme c-axis compressibility anisotropy ($B_c \approx 556$ GPa vs. $B_a \approx 997$ GPa), inducing periodic stacking faults in the R-S-R-S* block sequence and layer tilting [2]. Above 25 GPa, both features revert, restoring $P6_3/mmc$ as cumulative strain anneals faults. No such low-pressure stacking disorder or $P6_3/mmc$ → P31m transition is reported in $PbFe_{12}O_{19}$ or hexaferrite analogs, highlighting sample-dependent shear effects (e.g., defects/non-hydrostaticity). Equation-of-state analysis confirms $B_0 \approx 254$ GPa. These findings uncover transient pressure-tuned disorder in layered ferrites, with implications for multiferroic tuning [3].

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