

MS27 Minerals and Materials Under Extreme Conditions

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Comprehensive determination of the high-pressure structural behaviour of BaTiO₃

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Abstract

We have mapped the phase diagram of the archetypal ferroelectric material BaTiO₃ more extensively than previous attempts using high-pressure neutron-powder diffraction.[1] The mapping of the phase diagram has been performed using isothermal compression at fixed temperatures (175, 225, 290, 480 K) within each of the known crystallographic phases, up to ~6 GPa using a large volume press. The crystallographic structure of each phase has been measured, and using the unique information neutron diffraction provides we have determined the absolute atomic displacements of all atoms within the cell, obtained detailed information on the order of the phase transitions observed, and the behaviour of the ferroelectric dipole moment.

References

[1] Bull C.L. et al Materials Advances, 2,6094 (2021)

Phase Diagram of BaTiO₃

