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Crystal structure changes in $BaTiO_3$.

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The crystal structure of $BaTiO_3$ changes at the transition temperatures, where it undergoes a transformation from cubic to tetragonal to orthorhombic to rhombohedral as is well known (Mason, 1950). The figures used in nearly all modern textbooks (Jona & Shirane, 1962) describing this phenomenon are unfortunately correct in relative symmetry and polar direction but incorrect in relative cell dimensions.

The errors are probably caused by inaccurate drafting in the original figure describing the transformations, which errors have been retained in all subsequent reappearances. The visualization in a two-dimensional drawing of a skewed three-dimensional lattice obviously is not an easy matter.

This communication presents a corrected figure (Fig. 1) of these transformations.

Fig. 1 has been constructed from the primary data published by Kay & Vousden (1949). The changes in lattice constant, which experimentally amount to approximately 0·5 %, have been exaggerated by a factor of about 20, as in the original figure, to clarify the changes. Furthermore the volume expansion with temperature, which should be superimposed on the phase transformations, changing the scale of the figures slightly, has been neglected. Similarly the slight changes with temperature within each phase have been neglected. In the figures the heavy arrows indicate the direction of the spontaneous polarization in each phase and consequently also the direction of elongation.

References

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KAY, H. F. & VOUSDEN, P. (1949). *Phil. Mag.*, ser. 7, **40**, 1019.

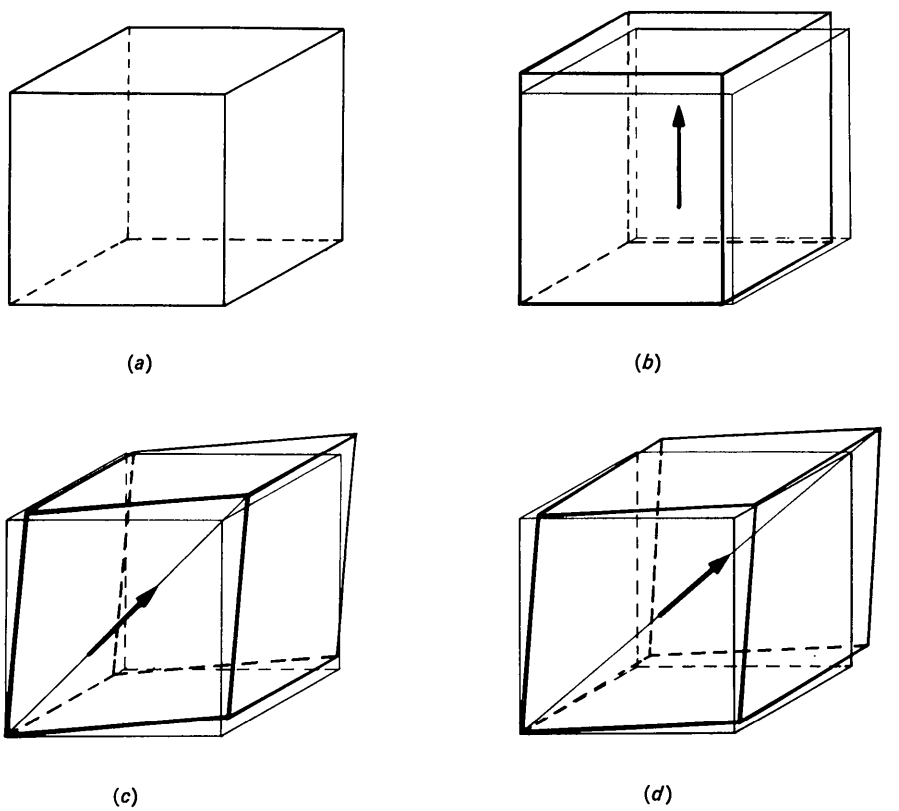

Fig. 1. Unit cells of the four phases of $BaTiO_3$. The original cubic cell is shown for comparison in each case. The arrows indicate direction of elongation and polarization. (*a*) Cubic, stable above 120 °C. (*b*) Tetragonal, stable between 120 °C and 0 °C. Elongated along a cube side. (*c*) Orthorhombic, stable between 0 °C and −90 °C. Elongated along a surface diagonal (two cube sides). (*d*) Rhombohedral, stable below −90 °C. Elongated along a body diagonal (three cube sides).