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Shifts: 12	Local contact(s): Gavin Vaughan	
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Report:

3DXRD data were collected on the tetragonal electroceramic BaTiO₃ (BT) at zero field and during a subsequent electrical hysteresis loop in order to determine orientations, lattice strains and volume fractions of thousand individual ferroelectric domains. These far-field grain centre maps have been complemented by a spacefilling near-field grain map at zero field, see the figure. The data is analysed to determine whether grains of similar orientation embedded in different environments undergo the same deformation, i.e. whether it is the orientation and/or the local environment that dictates the macroscopic behaviour of the material. Powder diffraction experiments have shown that the direction of maximum lattice strain within tetragonal electroceramics under applied field does not coincide with the single crystal ferroelectric polarization direction [1,2]. This observation is in contradiction to accepted theory in the area [3], which suggests that for tetragonal systems the maximum strain should be observed along the [001] polarization axis. It is currently unknown if this discrepancy arises from insufficiencies in the applied theory, or if complex medium length-scale inter-granular stresses cause unexpected unit cell distortions. The present grain-resolved data on a statistically significant number of grains allows us to shed light on these fundamental questions.

[1] J. L. Jones et al., Applied Physics Letters 90, 172909 (2007).

[2] J. E. Daniels et al., Journal of Applied Physics 101, 094104 (2007).

[3] D. Damjanovic, J. Am. Ceram. Soc. 88, 2663 (2005).

Figure 1 Preliminary grain map of BT from which grain neighbour relations can be derived.

