Exploring domains compatibility in polycrystalline ferroics

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Polycrystalline ferroics in either bulk or thin film constitute the basis for many of today's devices across a range of applications, including sensors and non-volatile memory devices; due to their low-cost and fast preparation time scales. The key characteristic of ferroic materials is the development of equivalent ground states, domains, that form to minimise the system's free energy. The reversible switching of these domains is what enables ferroics' functionality, and their configuration (or pattern) greatly influences the final properties of a ferroic.

Polycrystalline ferroics have intricate domain patterns where, the collective behaviour of the individual domain patterns is what ultimately determines the material's properties. Although domain coupling across grains has been already reported[1-3], the actual mechanisms allowing this is not yet fully understood; due to the complicated nature of the samples where other factor such as grain size and processing parameters impacts the final domain size and configuration. This level of knowledge is even more crucial when considering possible interaction or reorganisation of different domain patterns under the application of external stimuli. Thus, it is clear that in order to optimize our use of such microstructured ferroics for future technological applications, it is imperative to have a better understanding of domains' behaviour across grain boundaries in a static and dynamic manner.

In this study, the compatibility and coupling of selected domain pattern across different grains is explored, as well as their behaviour under heating cycles through the Curie Temperature (Tc) (ferroelectric-paraelectric phase transition). Aspects such as pinning, domain nucleation and domain re-orientation are also analysed. This is done experimentally by cutting lamellae from polycrystalline $BaTiO_3$ (BTO), giving the freedom to adopt a stress-free configuration, resembling more a thin film. The grains are initially characterized by electron backscatter diffraction (EBSD), followed by thin lamellae fabrication of selected grains with different junctions (containing 1 - 3 grain boundaries) by focused ion beam (FIB) and characterization by transmission electron microscopy (TEM) techniques including in-situ heating. An example of a lamellae and local EBSD analysis is shown in Fig. 1; while Fig. 2 shows an example of a heating the sample up to Tc. The data obtained is then rationalised in terms of crystallographic theory of martensite in order to understand and predict the final domain configuration of a grain within a grain junction.

We demonstrate that in the case of a lamellar polycrystalline samples, the relaxation of out-of-plane constraint gives rise to an underdetermined set of linear equations in the volume fractions of crystal variants. Additional inequality constraints on the volume fractions lead to (non-unique) solutions, indicating that groups of twinned grains in lamellae can form stress-free domain patterns. Since the constraint is much less than that of the bulk, a reorganisation of the bulk domain structure during heating and cooling of a lamella extracted from the bulk is likely.

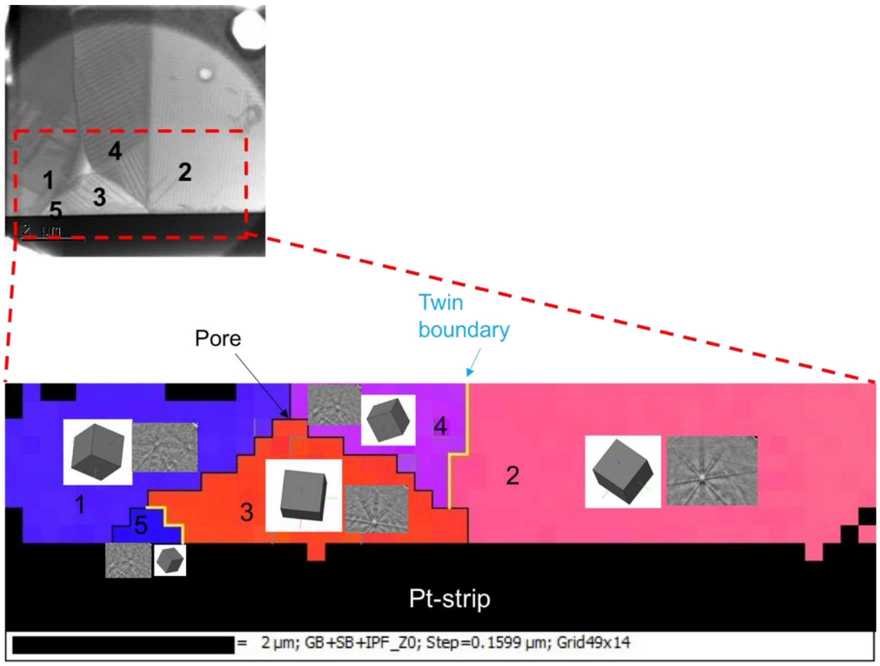

Figure 1. EBSD of $BaTiO_3$ lamella (Out-of-plane)

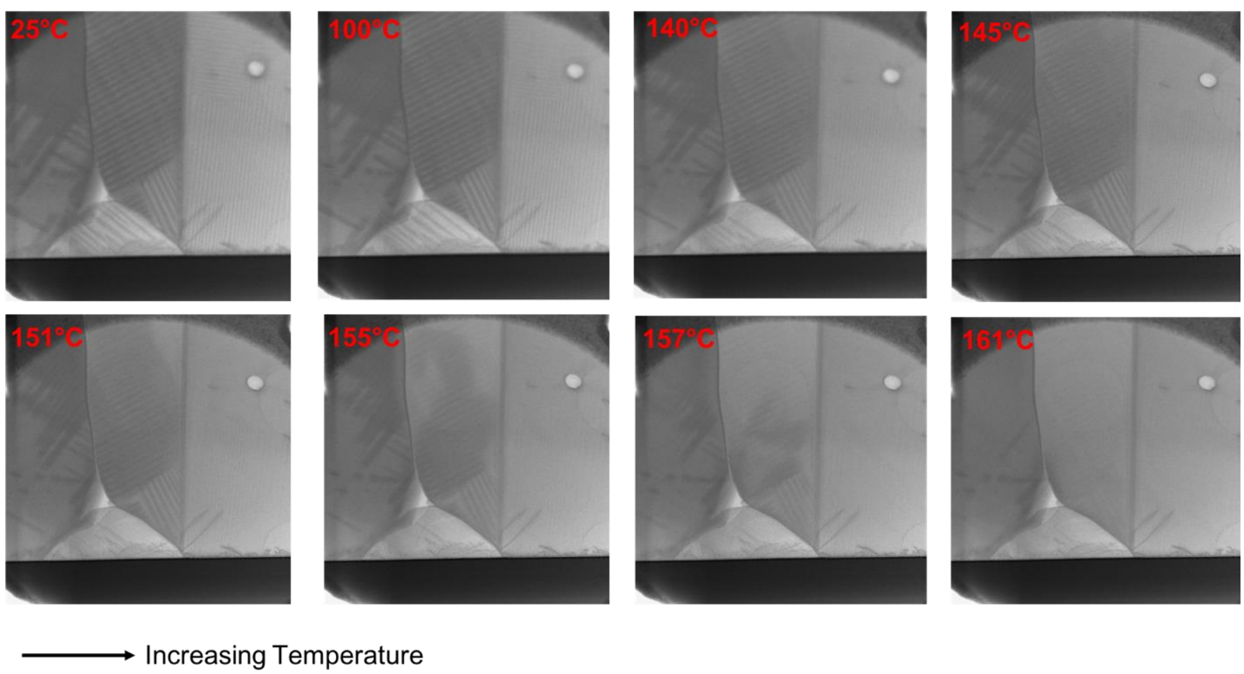

Figure 2. In-situ heat cycle 1 at 1°C/sec.

[1] Y. Ivry et al., 24, 35, 5567 - 5574, (2014)
[2] Y. Ivry et al., Adv. Funct. Mater, 2011, 21, 1827 - 1832 (2011).
[3] Gruverman et al., J. Vac. Sci. Technol. B14, 602.