

## Impact of Electric Fields on Grain Boundary Atomic and Electronic Structures

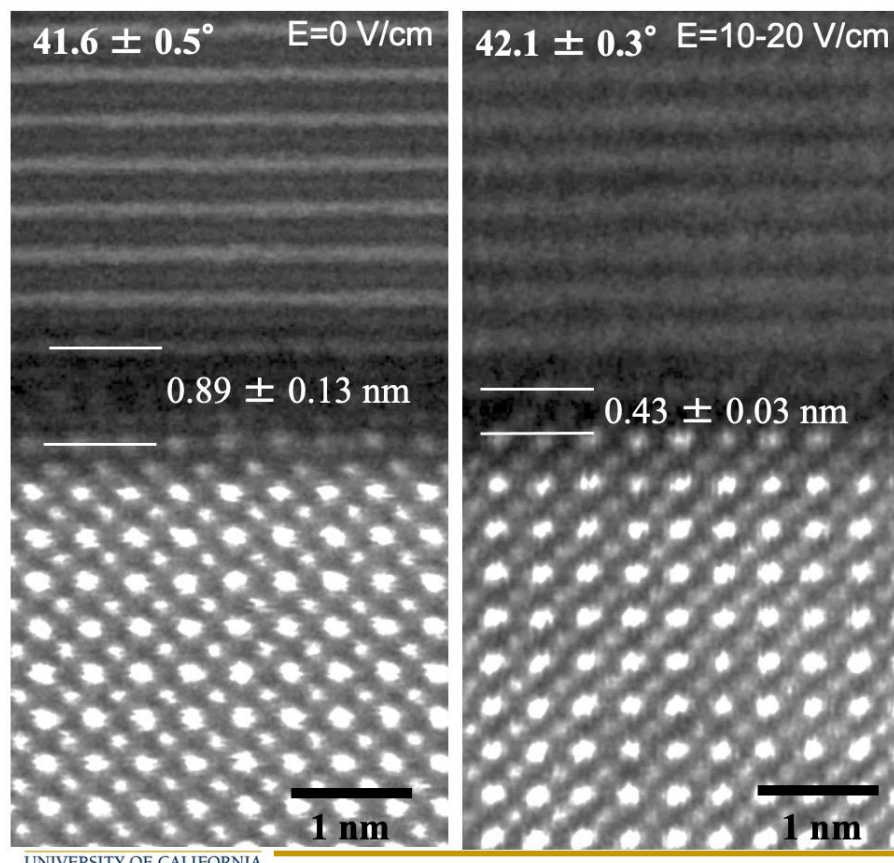
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Electric field assisted sintering, which includes Spark Plasma Sintering and Flash Sintering, has demonstrated the feasibility to accelerate densification of powder compacts, lower processing temperatures, and suppress or enhance grain growth [1]. A remaining fundamental question is how an applied electric field, in the absence of any appreciable current flow, affects grain boundary formation and the resulting interfacial microscopic degrees of freedom, i.e., local atomic interface structures.

For this study (100) twist grain boundaries of SrTiO<sub>3</sub> were diffusion bonded at 1450°C either in the presence of absence of externally applied electrostatic fields. High-angle annular dark-field (HAADF) scanning electron microscopy (STEM) imaging was carried out in conjunction with energy-loss near-edge fine structure (ELNES) analysis to characterize the atomic and electronic grain boundary structures as a function of applied electric field. It was found that for nominal electrostatic field strength between 20V/cm and 170V/cm s applied in the direction perpendicular to the grain boundary plane the interface expansion was only around 0.4 nm, while a grain boundary width closer to 0.9-1.0nm was detected after diffusion bonding in the absence of an applied electric field (see Figure 1). However, for field strength as high as 500 V/cm and 1500V/cm applied parallel to the grain boundary plane changes in interface expansion between the negative and positive electrode side were observed. Initial ELNES results suggest a migration of oxygen vacancies within the applied electric field likely coupled with cation diffusion that may have caused unmixing and potential dissociation of SrTiO<sub>3</sub> close to the negative electrode. Additional energy-dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy experiments are underway to confirm this hypothesis.

The experimental results may suggest the feasibility to trigger grain boundary transitions with applied electrostatic fields during processing of insulating ceramics.



**Figure 1.** HAADF-STEM images of (100) twist grain boundaries in SrTiO<sub>3</sub> diffusion bonded in the absence (left) and presence of an externally applied nominal electric field strength of 10-20 V/cm. Figure reproduced with permission from [2].

#### References

- [1] W. Rheinheimer, M. Fülling, M.J. Hoffmann, Grain growth in weak electric fields in strontium titanate: Grain growth acceleration by defect redistribution, *Journal of the European Ceramic Society* **36** (2016) 2773–2780.
- [2] L.A. Hughes, M. Marple, K. van Benthem, Electrostatic fields control grain boundary structure in SrTiO<sub>3</sub>, *Applied Physics Letters* **113** (2018) 041604.
- [3] L.A. Hughes, K. van Benthem, Effects of electrostatic field strength on grain boundary core structures in SrTiO<sub>3</sub>, *Journal of American Ceramic Society* **102** (2019) 4502-4510.
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