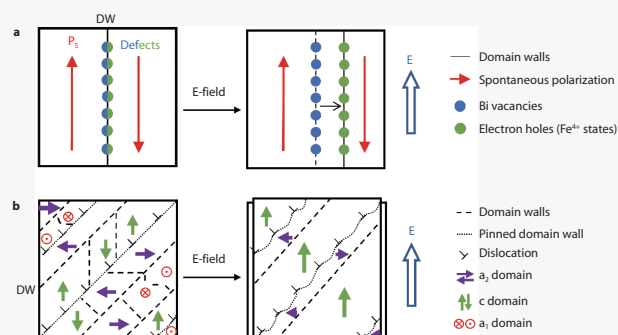


Defects in motion

Lisha Liu*

Defects play a critical role in tuning the macroscopic of ferroelectrics. In particular, their induction, their intrinsic characteristics, and their motion with the applied field during functioning of ferroelectrics are main research focuses. Specific attention to their dynamics and interactions with that of the ferroelectric domains should be paid in the future study.



Crystalline defects appear when the perfect order of the lattice or ideal arrangements of atoms, molecules, or ionic groups is destroyed, which is inevitable during crystal growth, thereby impacting material functionalities, either in a reinforcing or unwanted way. For functional ferroic materials, natural interfaces called domain walls form, which separate regions of different orientations of a specific order (such as magnetic, ferroelastic, or ferroelectric) in the material. These, including phase boundary, grain boundary, and/or domain boundary, can be reckoned as two-dimensional defects. During functioning of ferroic materials, phase transformation and/or dynamic motion of domain walls occur with external stimuli like electric fields or stress. Therefore, domain engineering, phase boundary construction, and grain engineering has long been the most considered effective strategies to enhance the performance of ferroic materials. Meanwhile, lower-dimensional defects, including point defects, defect dipole, and line defects, are another crucial dimension to be considered to tune functionality, since their motion greatly interact with the domain wall dynamics under external stimuli. In all, defect engineering (here we refer to one- and two-dimensional defects) and its coupled motion with order parameters is an interesting topic that has attracted significant attention for functional oxides.

In *Nature Materials* and *Nature Communications*, Tadej Rojac and colleagues at the Institute of Josef Stefan (IJS) have shown that point defects in BiFeO₃, such as Bi vacancies or oxidized/reduced Fe or O vacancies, can gather at the ferroelectric domain walls. When the field is applied, the defects move

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with the domain wall (as shown by the schematic in Fig. 1a), impacting the pinning and depinning of domain wall dynamics^[1–2]. This was visualized by contemporary aberration-corrected transmission electron microscopy (TEM), as this atomic resolution is ideal for characterizing crystalline defects and following the ferroelectric switching process via special in situ sample cells. Many similar works have used this technique in the same way, which enables direct insights in the pinning or more complex behavior of defects in such materials^[3–6]. Thus, defect motion should be considered in designing the properties of crystalline materials, such as designing a strategy to obtain reversible strains as high as 0.75% in BaTiO₃ single crystals, where the polarization and defect dipole show the same symmetry, which is known as the symmetry conforming principle^[7].

Science and Nature Communications have recently proposed the replacement of lower dimension point defects by line defects, or dislocations, via mechanical transformation (also known as creep), to tune ferroelectric properties^[8–9]. Via scanning electron microscopy electron channeling contrast imaging (SEM-ECCI), domain nucleation at dislocations and interactions between domain walls and dislocations, which can be described by a local pinning force, were observed. This local pinning force acts in conjunction with a macroscopic restoring force on domain dynamics, i.e., domain variants selection by dislocation pinning which is in favor of reversible domain switching (see the schematic in Fig. 1b). This causes a significant enhancement in the electromechanical properties. Surprisingly, a 5-fold increase in the dielectric permittivity and a 19-fold increase in the piezoelectric coefficient have been demonstrated in a BaTiO₃ single crystal. In 2022, the introduction of ultra-high density dislocations (three orders higher than in normal ceramics) through enhanced system entropy was used to achieve ~70% improvement in fracture tough-

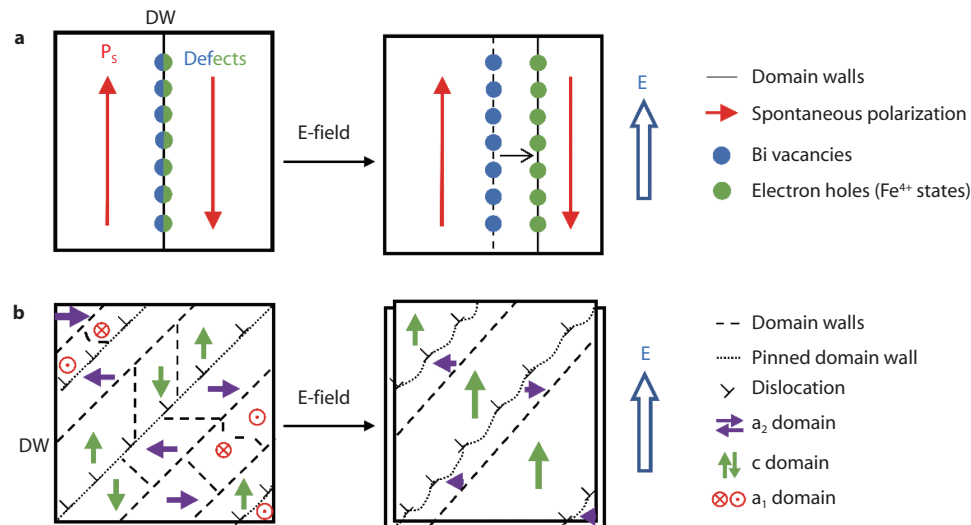


Fig. 1 Schematic of crystalline defects and domain walls in ferroics during dynamic processes. **a** Domain wall dynamics with point defects^[1]. Copyright 2020, Springer Nature. **b** Domain wall dynamics with line defects (dislocations)^[8]. Copyright 2021, AAS.

ness of pyrochlore ceramics^[10–11]. The introduction of dislocations provides a unique opportunity to modify the movement of the domain wall at specific points and is thus an exciting alternative to conventional approaches of point defect engineering.

What is worth noting is that although the role of both point defects and line defects in ferroics has been proven to be significant and effective, the engineering and even the observation, with the development of related techniques, is far from mature. The latter seems to be the foremost problem to be solved so far, in particular the direct observation/imaging of defects in a larger mesoscopic scale. In particular, with enhanced resolution and bulk detection sensitivity. In 2018, Simons et al. reported the use of X-ray diffraction imaging to directly study the domain patterns inside different grains of perovskite BaTiO₃ ceramics. The process of domain wall movement (i.e., domain wall flipping) and the long-range strain field (extending from the domain wall) that is experienced in the interior during the flipping process can also be clearly demonstrated^[12]. Later in 2020, Wallentin et al. used in situ X-ray imaging to study the evolution of striped ferroelastic domains in metal halide perovskite CsPbBr₃ with increasing temperature, and the distribution of local stress near the domain wall in the material under ferroelastic domain evolution was aptly visualized^[13]. The above research results reveal that direct mesoscopic quantification and visualization of the dynamic interactions of defects and domain walls in motion are technically possible. In the future, three-dimensional visualization of defects or dislocations (or their local strain fields), in particular to the bulk, are expected to significantly assist the understanding of defects, as well their interaction with ferroelectric domain dynamics. Thus, more intuitive research can facilitate an understanding of the distribution, concentration, interaction, and impact on the formation of order parameters of both point defects, defect dipoles, and dislocations, as well as their interactions with the material order parameter during dynamic processes.

All in all, to continually push the limits of the electromechanical, dielectric, and electrochemical properties of function-

al oxides, the principles of prevention/creation and stability/motion of defects of all dimensions are crucial in material science.

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■ CONFLICT OF INTEREST

The authors declare no conflict of interest.

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Biography



Lisha Liu is working at Nanjing University of Science and Technology (NJUST), focusing on the research of high-temperature piezoelectrics (including single crystals, ceramics and films). She has rich experiences in synchrotron X-ray diffraction to analyse the domain physics and TEM for understanding local atomic structure within domains and at the domain walls.