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Mapping Orthorhombic Domains with Geometrical Phase Analysis

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Background incl. aims

Perovskite oxide compounds, with the chemical formula ABO3, constitute one of the most studied family of oxides due to its large variety of fascinating properties combined with their high degree of tunability. Although the prototypical perovskite lattice is cubic, additional structural distortions emerge when the ionic size ratio (A/B) deviates from one, thus lowering its symmetry. Among all the possible resulting space groups, the orthorhombic Pbnm lattice is one of the most common ones. For instance, most Vanadates, Nickelates, Iridates and Titanates share these particular lattice symmetries. The anisotropic unit cell of such compounds is characterized by in-phase octahedral rotations about one pseudocubic axis (the long orthorhombic one) and out-of-phase rotations about the other two pseudocubic ones; plus additional relative A-site displacements that feature a zig-zag pattern along the [110]PC direction.

When growing epitaxial heterostructures, the Pbnm lattice may nucleate differently oriented depending on how the unit cell is constrained by its neighboring epitaxial layers. When different orientations are equally energetically favorable, the presence of lattice domains with distinct orientations emerge, which in turn may lead to the presence of crystal defects. Retrieving all of this information is therefore paramount when designing novel heterostructures for electronic devices, as it will affect their resulting physical properties. For instance, improper ferroelectricity in artificial superlattices requires the long orthorhombic axis to be oriented out-of-plane. However, since the three pseudocubic axes are in most of the cases very similar in length, it is typically challenging to extract this information from conventional X-ray diffraction analyses.

Methods

In this contribution, we present a very simple and fast approach devoted to map Pbnm lattice domains.1 It is based on using the conventional geometrical phase analysis (GPA) but in a non-conventional manner. Since the relative zig-zag displacements of the A-site cations double the unit cell length along the long orthorhombic axis, they feature additional half-order reflections in the Fourier Transform (FT) pattern of aberration-corrected STEM images. The strategy behind our methodology consists then on using the conventional aperture settings used for regular strain mapping (centered in the (001)PC and (100)PC or (010)PC reflections), but this time including the {(1/2) 0 1}PC or {1 0 (1/2)}PC reflections within the selected aperture area as well. When these particular aperture settings are used, additional fringes (related to the A-site relative displacements) appear in the exy and rxy maps only in those areas contributing to the emergence of these half-order reflections in the corresponding FT pattern.

Results

As a showcase of the versatility and robustness of this methodology, we further exploit this approach to determine the structural parameters that set the lattice orientation and associated domain distribution in rare-earth nickelate compounds. For this, we have analyze the domain distribution in a series of rare-earth nickelate heterostructures grown under distinct structural constraints. Although we will show that the resulting lattice orientation and domain distribution mainly depends on the in-plane normal epitaxial strain, we will also demonstrate how shear strain and interfacial structural connectivity are also very relevant, and should not be neglected when designing novel heterostructures.1-3

Finally, we will also show that this methodology is not restricted to Pbnm domain mapping, but can also be exploited to identify some specific lattice defects or domain boundaries that are otherwise very challenging to localize. Further, beyond Pbnm compounds, it can be adapted to map other types of structural periodicities from other space groups that also also render half-integer reflections in the FT patterns of STEM images.

Conclusion

To summarize, in this contribution we will first present a fast, robust and versatile methodology that is very useful to map Pbnm lattice domains. Second, we will discuss how we have applied this to identify key structural parameters that influence domain distributions in epitaxially-grown Pbnm compounds. Finally, we will also comment about other possible scenarios where this methodology can be also useful to track and map periodic structural distortions that render half-integer reflections in the FT patterns of STEM images.

Keywords:

STEM, GPA, Perovskites, strain, mapping.

Reference:

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