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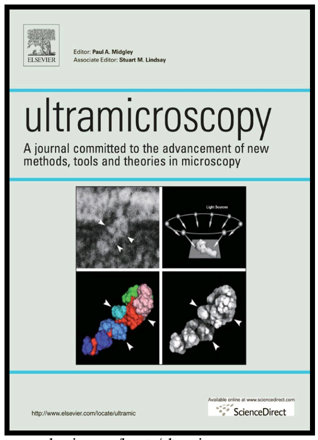

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Quantification by aberration corrected (S)TEM of boundaries formed by symmetry breaking phase transformations

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Abstract

The present contribution gives a review of recent quantification work of atom displacements, atom site occupations and level of crystallinity in various systems and based on aberration corrected HR(S)TEM images. Depending on the case studied, picometer range precisions for individual distances can be obtained, boundary widths at the unit cell level determined or statistical evolutions of fractions of the ordered areas calculated. In all of these cases, these quantitative measures imply new routes for the applications of the respective materials.

Keywords: aberration correction; quantification; alloys; oxides; phase transformation; pico

Introduction

Crystal defects in materials are well known for their importance for the behavior of the material. From point defects providing the colors in precious stones over moving dislocations dictating the mechanical behavior of metals to precipitates affecting the magnetic properties in alloys, in all cases the defect structures are primordial to the functionality of the material. To understand, predict and possibly tune these parameters it is crucial to understand the exact atomic structures of these defects is essential. Indeed, because of lattice relaxations, when compared with the perfect matrix, small displacements or rearrangements of atoms can be expected at the sites of the defects. Depending on the system, such effects can be seen at the nanoscale, but in some cases they are limited to the picorange or to minor changes in chemical concentration. In this context aberration corrected transmission electron microscopy (AC-TEM) with image resolutions below the Ångstrom and, more importantly, precisions in the picorange, becomes an important tool [Haider et al., 1998; Xu et al., 2005; Bals et al., 2006; Urban, 2008; Jia et al. 2008]. Also, Z-contrast quantification in an AC-TEM can yield information on individual atomic site occupations [Pennycook et al., 1991; Van Aert et al., 2011; Martinez et al., 2014].

In the present work the focus will be on crystallographic boundaries generated by symmetry breaking phase transformations. Four examples of recent work in this field will be reviewed, two on polar oxide systems, $CaTiO_3$ and $LiNbO_3$, and two on metals, one with a diffusive (Co-Pt) order-disorder and one with a displacive martensitic (Ni-Ti) phase transformation. In the oxide systems as well as the martensite the aim is to measure local atom displacements