Z-contrast STEM imaging of B cation ordering and microstructure of Sr_2CrReO_6 double perovskite thin films

C. Magén[1,2]*, M. Varela*[2]*, S. J. Pennycook*[2]*,*
J. Orna[1,3]*, L. Morellon*[1,3]*, P. A. Algarabel*[3]*, M. R. Ibarra*[1,3]

[1] *Instituto de Nanociencia de Aragón, Universidad de Zaragoza, 50009 Zaragoza, Spain*
[2] *Oak Ridge National Laboratory, Oak Ridge TN 73831, USA*
[3]*Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza-CSIC, 50009 Zaragoza, Spain*
cmagend@unizar.es

Half-metallic compounds present a great potential for room-temperature applications at room Spintronics. Ferrimagnetic double perovskites (DP) with formula unit $A_2BB'O_6$) are candidates to exhibit half-metallicity and high Curie temperatures based on a modified perovskite structure where the $BO_6/B'O_6$ octahedra are arranged in a superstructure of two interleaving fcc sublattices antiferromagnetically coupled [1]. Sr_2CrReO_6 (SCRO) is a metallic ferromagnetic DP with one of the highest Curie temperature (T_C=625 K) [2]. SCRO has a experimental saturation magnetization of M_S=1.38 μ_B/f.u (the theoretical value is 1 μB/f.u) [3], but the existence of antisite (AS) defects at the B/B' sites can reduce this value and also destroy the half-metallic nature of the material.

The controllable growth of high-quality epitaxial films of SCRO ordered double-perovskite with high T_C and full magnetization is required for electrodes in spintronic devices [4,5,6]. In this work we report the Z-contrast STEM characterization of the chemical ordering and microstructure of epitaxial SCRO deposited on $SrTiO_3$ (001) substrates by pulsed laser deposition (PLD). The growth conditions can be found elsewhere [7]. High resolution scanning transmission electron microscopy (HR-STEM) were performed in the VG Microscopes HB501UX and HB603U operated at 100 kV and 300 kV, respectively and both equipped with a Nion aberration corrector.

High resolution annular dark field (ADF) STEM image of a cross section specimen of SCRO is depicted in Figure 1. In this image we can clearly perceive the cationic ordering in the B sites due to the Z-contrast. The intensity profile of the image evidences the presence of the three elements; i.e. Sr (A site), Re and Cr (B, B' sites). Figure 2 displays a Z-contrast image of the SCRO film in the proximity of the substrate, which shows an excellent epitaxial growth of the SCRO layer in the early stages of the growth and a defectless unrelaxed interfase. The epitaxy relations in this stage of growth are STO (111) [1-10] // SCRO (111) [1-10]. At a thickness of approximately 4-5 nm we can observe the formation of two sets of twins in the shape of planar grains parallel to the substrate plane with two alternating orientations. One corresponds with the same orientation as the substrate (i.e. the twin present in the first nanometers of the film), the other with the *a* axis rotated ~110º clockwise in the image. The orientation of the second set of twins corresponds to a rotation of the SCRO crystal of 180º around the (111) axis. Therefore, the epitaxy relation of the second twin with respect to the first one (i.e. with respect to the substrate is STO (111) [1-10] // SCRO (111) [100]. Z contrast is a powerful tool to characterize the chemical ordering in DP. The effect of the formation of twin boundaries can be observed in Figure 2(b). While in the upper boundary the B superstructure is conserved through the boundary (thick lines indicate the Re columns and thin lines are Cr columns), the lower boundary creates an AS boundary.

References:

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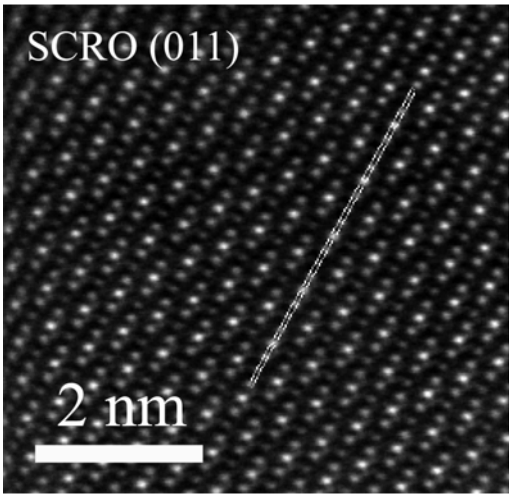
Figures:



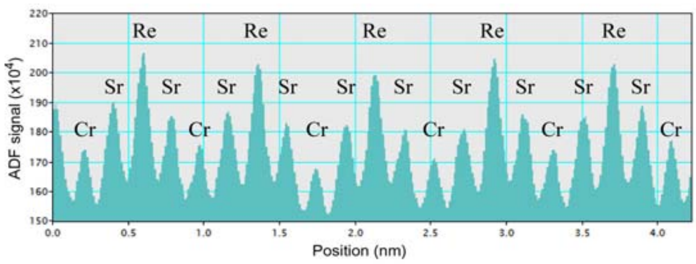


Figure 1. Z-contrast STEM image of one of the twins of the SCRO film oriented along the zone axis (110) where the B cation ordering can be observed and intensity profile (VG603).

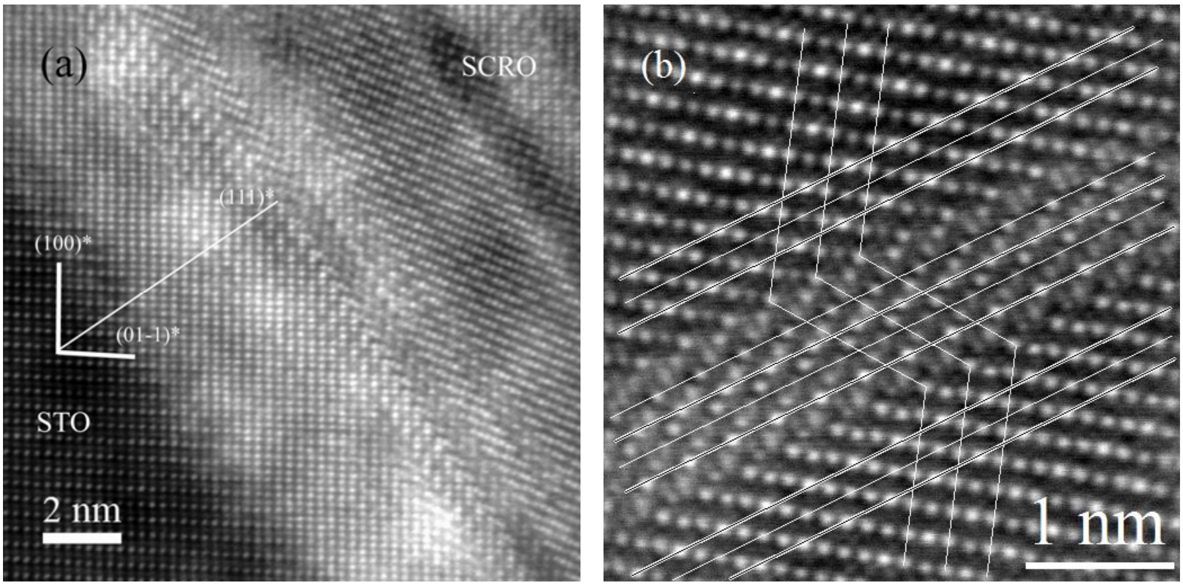


Figure 2. (a) VG 501 High resolution Z-contrast STEM image of a cross section SCRO specimen grown on STO (111) (VG501). (b) Fourier filtered image of a twin boundary in SCRO (VG603).