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Orientation of the charge-density-wave chains in thin films of $Rb_{0.30}MoO_3$

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Abstract

The in-plane orientation of the charge-density wave (CDW) chains in thin films of $Rb_{0.30}MoO_3$ has been investigated by X-ray diffraction and electron microscopy (SEM and TEM). On $SrTiO_3(100)$ substrates, the CDW chains align with the principal axes of the substrate surface lattice. The CDW chains run parallel to the long dimension of grains of $Rb_{0.30}MoO_3$.

Keywords: charge-density waves, thin films, X-ray diffraction, transmission electron microscopy

1. Introduction

Charge-density waves (CDWs) occur in materials that have a strongly anisotropic crystal structure [1]. Upon cooling down, such materials exhibit a Peierls transition to a state with a periodic modulation of the charge density. This CDW state results in remarkable electrical transport properties. If an electric field larger than a threshold value is applied, the CDW can slide through the crystal. CDWs have been studied extensively in bulk crystals of $NbSe_3$, TaS_3, and the blue bronzes $A_{0.30}MoO_3$, with A one of the alkali atoms K, Rb, or Cs [2,3].

Recently, we have reported the growth of thin films of $Rb_{0.30}MoO_3$ by pulsed-laser deposition [4]. The crystal structure of this material is monoclinic, space group C2/m, with lattice parameters a=18.54 Å, b=7.55 Å, c=10.04 Å, and β=118.52 Å [5]. Below 182 K, CDW transport can occur along the *b*-axis, parallel to chains of MoO_6 octahedra.

Our thin-film efforts are motivated by the interest to study electrical transport in mesoscopic CDW devices, i.e., structures with dimensions less than the CDW phase coherence length. For this purpose, films are patterned by lithographic techniques [6]. Since sliding of CDWs only occurs along the *b*-axis, the orientation of this axis must be well defined for electrical transport studies. All films are granular, with the *b*-axis parallel to the substrate plane [4]. Here, we study the alignment of the CDW chains *within* this plane for films on $SrTiO_3(100)$ substrates.

2. In-plane orientation of the CDW chains

The morphology of blue-bronze films has been studied with scanning electron microscopy (SEM). For most of the substrate types used, films consist of micron-sized grains that have the *b*-axis randomly oriented within the substrate plane. On $SrTiO_3$, in-plane alignment to the substrate occurs. Figure 1(a) shows a SEM image of a film grown on $SrTiO_3(100)$. Elongated grains of typically 1 μm length are visible. The grains appear to be predominantly oriented into two perpendicular directions. From the known orientation of the substrate edges, we find that the long dimension of the grains is parallel to either the [010] or the [001] axis of the substrate.

The in-plane orientation of the CDW chains has been studied with an X-ray 4-circle diffractometer. Films are aligned such that the ϕ-axis of rotation is perpendicular to the substrate plane. A blue-bronze $(\bar{2}21)$ reciprocal vector, which is a linear combination of the $(\bar{2}01)$ vector (parallel to the axis of rotation) and the *b*-axis, is then brought into the reflection condition. By rotation over ϕ, the distribution of orientations of the CDW chains within the substrate plane is obtained. The result is shown in Fig. 1(b). The CDW chains are predominantly oriented into two perpendicular directions. The grains appear to be aligned with the CDW chains parallel to one of the principal axes of the substrate surface lattice.

3. Orientation of the *b*-axis in a single grain

Combination of Figs. 1(a) and 1(b) leads to the conclusion that the CDW chains in a single grain are directed either parallel or perpendicular to its long dimension. The orientation of the *b*-axis in a single grain can be determined from high-resolution top-view TEM images. Figure 2 is such an image for a single grain of the same film on $SrTiO_3(100)$ that is shown in Fig. 1. The inset shows one grain as a whole. Unit-cell resolution is obtained by zooming in on the area marked by the white square. The grain boundary, visible in the right part of the main figure, appears to be quite sharp. An electron-diffraction pattern of the grain confirms that this indeed is a $(\bar{2}01)$ grain. It also shows that

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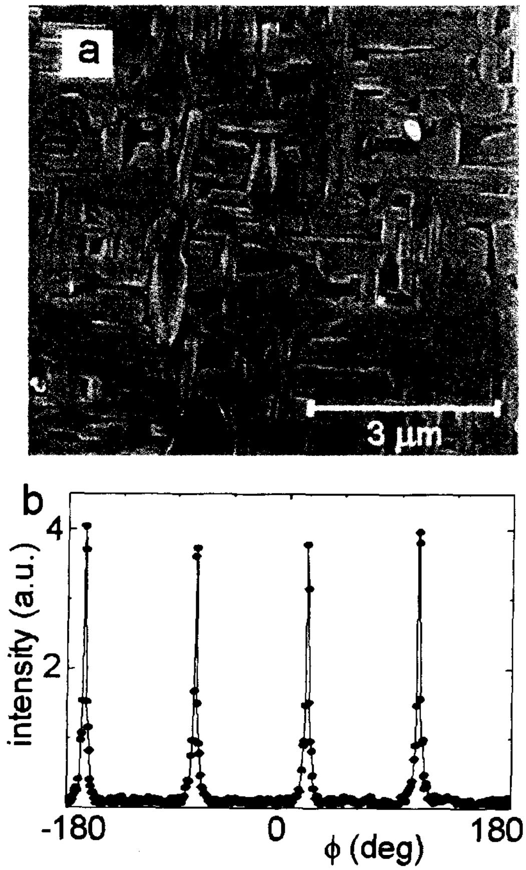

Figure 1: *a) SEM picture of a film grown on $SrTiO_3$(100), showing the two perpendicular grain orientations. b) X-ray scan of this film, revealing the in-plane distribution of the CDW chains. The positions of the peaks coincide with the positions of the reflections from the crystalline substrate (not shown).*

b is directed as indicated in the figure. The spacing between lattice planes in the vertical direction is 3.8 Å, which corresponds to $|b|/2$. Thus, we find that the *b*-axis is parallel to the long dimension of the grain. This observation is supported by pictures made of other grains in the same film. Note that the grains in this film have a shape that is similar to the shape of bulk blue-bronze crystals. Such crystals also grow with the *b*-axis parallel to the long dimension.

4. Conclusion

On $SrTiO_3$(100) substrates, the CDW chains in $Rb_{0.30}MoO_3$ films are aligned with the principal axes of the substrate lattice. Top view TEM images show that the CDW chains in a single grain are parallel to its long dimension. This information is important for electrical-transport measurements on lithographically patterned structures.

Note that the CDW chains can be predominantly oriented into one direction by using the (510) cut of $SrTiO_3$. X-ray measurements show that in films grown on this substrate approximately 90% of the CDW chains can be aligned with the [001] principal axis of the substrate [4].

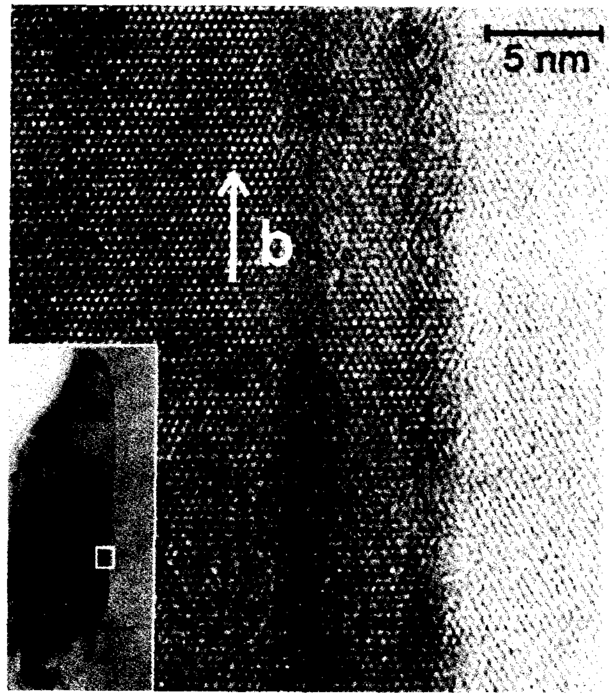

Figure 2: *Top-view TEM image of an elongated $Rb_{0.30}MoO_3$ grain. The inset shows the shape of the grain. The position at which the high-resolution image is made is indicated by the white square. The b-axis appears to be parallel to the long dimension of the grain.*

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