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Interface structure in high-T_c superlattices

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Abstract. We have studied the structure of high-T_c superlattices and films through refinement of the x-ray spectra. The results indicate that interdiffusion, layer thickness fluctuations and strains are present and cannot be neglected.

The dimensionality of superconductivity in high-T_c materials is a crucial issue to help reveal the underlying physics. Regarding this point it is important to ascertain if a one-unit-cell (UC)-thick $RBa_2Cu_3O_x$ (RBCO) film is superconducting. It has been reported [1] that a 1 UC thick YBCO film is superconducting when deposited between PrBCO layers. The YBCO/PrBCO superlattice system has also been used as a model to study the thickness dependence of T_c [2–4]. In both cases, the system being studied is not an isolated YBCO film, but a YBCO film surrounded by PrBCO. To understand the measured properties it is essential to determine the interface and film structure.

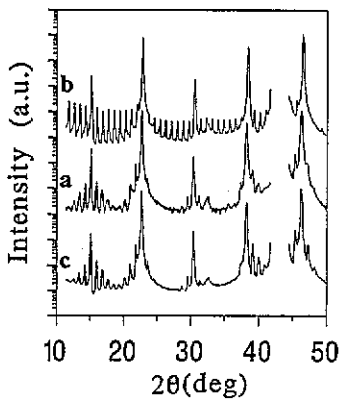

Figure 1. θ–2θ x-ray spectra of a 2000 Å thick YBCO(1 UC)/PrBCO(8 UC) superlattice: curve a, experimental spectrum; curve b, perfect superlattice calculation; curve c, refined spectrum. Spectra have been offset and the MgO(200) substrate peak has been erased for clarity.

Formerly we reported on the thickness dependence of T_c in PrBCO/YBCO/PrBCO trilayers [5] grown by DC magnetron sputtering [6]. We found that the system is not superconducting for films thinner than 15 Å$\simeq 1\frac{1}{4}$ UC. In order to analyse the structure of the interfaces we refined the x-ray diffraction spectra of superlattices grown by the same technique [7]. The refinement technique, which allows the introduction of disorder mechanisms in the structure model, has been described elsewhere [7, 8]. Figure 1 curve a shows the experimental θ–2θ diffraction spectrum of a YBCO (1 UC)/PrBCO(8 UC) superlattice. Figure 1 curve b

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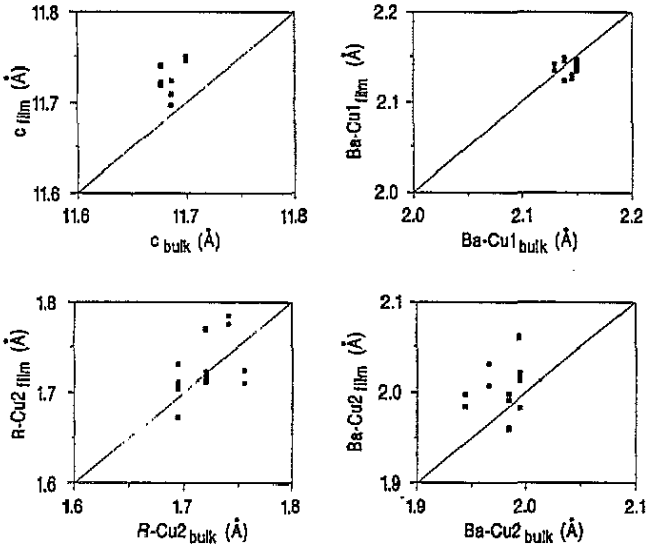

Figure 2. Interplanar distances in RBCO films versus interplanar distances in bulk materials for YBCO, PrBCO, GdBCO and DyBCO films. Vertical dispersion indicates variations between different films and different refinements for each film.

shows the calculated intensity assuming a 'perfect' superlattice with sharp interfaces and bulk interatomic distances. There is qualitative disagreement between the calculated and measured superlattice peak widths, positions, and relative intensities. Figure 1 curve c shows the refinement obtained after including interdiffusion between the R sites and layer thickness fluctuations in the structure model. The results indicate: (a) 30±5% interdiffusion of Pr in the Y sites for 1 UC thick films; (b) 1 UC thickness fluctuations around the 1 UC average thickness; (c) strains, which manifest themselves as deviations of the interplanar distances from the bulk values. These strains are also observable in thin films. In figure 2, we plot the interplanar distances and *c* lattice parameter refined for single films of YBCO, GdBCO, PrBCO and DyBCO, versus the bulk values. The *c* lattice parameter evidences an expansion of the film structure. The refinement indicates that this expansion does not occur in the Ba–Cu1 (Ba–CuO chains) distance. Although the scatter in the data does not allow a conclusive answer, this expansion seems to originate in the Ba–Cu2 (Ba–CuO_2 planes) distance which is the one governing the charge transfer mechanism (Cu2–apical oxygen).

In conclusion, RBCO films and superlattices are not ideal and structural disorder should not be neglected.

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