Physica C 185–189 (1991) 2069–2070
North-Holland

PHYSICA C

DISORDER AND SUPERCONDUCTIVITY IN $YBa_2Cu_3O_{7-\delta}/GdBa_2Cu_3O_{7-\delta}$ SUPERLATTICES

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The structure of *c*-oriented $YBa_2Cu_3O_{7-\delta}/GdBa_2Cu_3O_{7-\delta}$ superlattices is analyzed through refinement of the X-ray diffraction spectrum. This novel technique, similar in spirit to the well known Rietveld refinement of powder X-ray diffraction spectra, allows quantitative determination of the interfacial roughness. The results show that for these superlattices the roughness consists in step disorder of one unit cell around the average thickness of the layer and interdiffusion of 15 to 25% between the Y and Gd sites within one unit cell from the interface.

Superlattices of high T_c materials, in particular $YBa_2Cu_3O_{7-\delta}/PrBa_2Cu_3O_{7-\delta}$ (Y123/Pr123), are being used as a test ground to study the anisotropy of these compounds, i.e. the coupling between CuO layers.[1-3] The modulation and layer thickness dependence of the superconducting properties is the probe used to study this interaction. Since these properties could not only be affected by the coupling but also by the interface characteristics, like the partial interdiffusion of the trivalent ions, it is extremely important to characterize this interface.

We have used a new refinement technique[4] to study the structure of superlattices from their θ-2θ X-ray diffraction spectra (XRD). This technique, analogous to the well known Rietveld refinement for XRD of powders, allows quantification of interfacial properties such as roughness, atomic spacings and interdiffusion.

In this paper we present results on the structure of *c*-oriented Y123/Gd123 superlattices. The artificial structures were grown on single crystalline (100) MgO by DC magnetron sputtering from stoichiometric targets. The sputtering gas was a 90% Ar - 10% O_2 mixture and the pressure was 300 mTorr. During deposition the substrate was kept at ≈ 700°C and it was positioned outside the glow discharge area to avoid resputtering effects. All samples showed superconducting transitions at around 85K with little dependence on the layer thickness, as expected from the slight T_c dependence on composition of the bulk $Y_{1-x}Gd_xBa_2Cu_3O_{7-\delta}$ alloys.[5]

Figure 1 shows the experimental XRD spectrum, the simulated spectrum without disorder and the refined spectrum for a *c*-oriented [Y123 (4unit cells) / Gd123 (4unit cells)] x 21 superlattice. Superlattice satellite peaks are observed in the experimental spectrum around all the (00n) reflections. The existence of these peaks is usually taken as evidence of an excellent layering in the superlattice. However the striking difference between the satellite peak width and intensity in the perfect superlattice simulation and the experimental data clearly indicates that interfacial disorder has to be considered in order to determine the superlattice structure.

Two different interface disorder mechanisms were considered to model the interface: a) partial interdiffusion between the trivalent ion sites: this mechanism is expected to affect the relative intensity of the superlattice XRD peaks but not their width since it does not change the modulation length; b) steps of integer number of unit cells: this mechanism is expected to affect the superlattice peaks intensity and width since it affects the local periodicity of the structure. Therefore both mechanisms affect the XRD spectrum in different ways and can be refined

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Work supported by ONR grant #N00014-88K-0480.

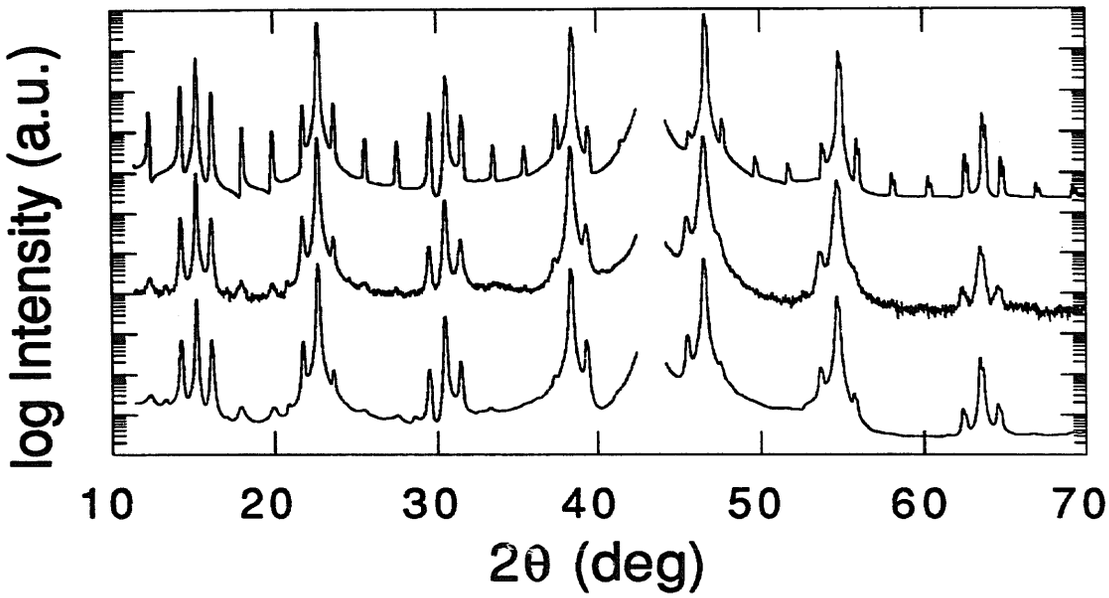

FIGURE 1

θ-2θ X-ray diffraction spectra for a *c* -oriented [$YBa_2Cu_3O_{7-\delta}$(4 unit cells)/$GdBa_2Cu_3O_{7-\delta}$(4 unit cells)] x 21 superlattice. Upper curve, calculated spectrum for a perfect superlattice; center curve, experimental spectrum; lower curve, refined spectrum including step disorder and interdiffusion at the interfaces. The curves have been offset by 3 decades and the MgO (200) peak at 42.9° has been erased for clarity. Full width at half maximum of the rocking curve around the (005) reflection at 38.4° is 0.35°.

independently.

The agreement of the refined and experimental spectra over 4 orders of magnitude of intensity is quite remarkable. The numerical results indicate interdiffusion in the first unit cell from the interface of 20% to 25% for an [Y123 (1unit cell)/Gd123 (1unit cell)] x 85 superlattice and 15% in the [Y123 (4unit cells) / Gd123 (4unit cells)] x 21 superlattice of figure 1. In both cases the step disorder is limited to 1 unit cell steps. These results imply that interdiffusion is playing an important role in the structure of high T_c superlattices and the layer thickness dependence of their physical properties.

ACKNOWLEDGEMENTS

We thank Prof. K. Kitazawa and Dr. T. Izumi for arranging the Tonen-UCSD collaboration

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