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In-plane orientation effect on the melting behaviour of YBCO thin film

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Abstract

By means of high-temperature optical microscopy (HTOM), a 60 °C gap in initial melting temperature between two $YBa_2Cu_3O_x$ (Y123) thin films was found *in situ*. Using these two films as seeds, liquid phase epitaxy (LPE) dipping experiments showed the same tendency in the melting behaviour. The in-plane orientation was detected by x-ray diffraction (XRD) pole figure. On the basis of results from HTOM, LPE and XRD, it was unveiled that the interface structure has a predominant influence on the melting mode. A semi-coherent interface suppresses not only the melting growth but also the melting nucleation, while an incoherent interface encourages both of them. (In this work, melting of YBCO refers to the peritectic decomposition of Y123.)

(Some figures in this article are in colour only in the electronic version)

1. Introduction

As a universal phenomenon in nature, the melting of a solid has been investigated both theoretically and experimentally for a long time [1]. It is well known that the melting of solids originates at a remarkably low temperature if their dimension is reduced. Meanwhile, with the development of nano-technology, more and more low-dimensional materials have found potential industrial applications. The loss of thermal stability could become one of the overriding obstacles against their further development and application.

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Table 1. The heating procedure for YBCO thin films in HTOM observations. The word 'limit' refers to the target temperature in each step, and 'holding time' means the duration that the system is held at the set value (the 'limit') when the temperature reaches this temperature point.

Sample	Heating rate (°C min^{-1})	Limit (°C)	Holding time (min)
A	80	930	3
	40	1020	3
	100	30	0
B	80	1010	3
	15	1060	3
	100	30	0

In recent years, a large amount of effort has been devoted to elevating the melting point of low-dimensional materials. After the first report by Däeges *et al* [2] in 1986, a superheating phenomenon was observed in many low-dimensional metal systems [3–5]. In most particle cases, the suppression of melting nucleation by epitaxial confinement at the interface is well accepted. Nevertheless, only partial epitaxial confinement has been mentioned experimentally in the two-dimensional (thin film) superheating so far [5]. More experimental results are much needed for further investigation.

As a good example of two-dimensional materials with great potential applications, such as second-generation coated conductor and microwave devices, $YBa_2Cu_3O_x$ (YBCO) thin films have attracted considerable interest. However, the study of thermal stability in YBCO thin films remained almost nil until the superheating phenomenon of the films was found [6]. As a good candidate seed for the preparation of REBCO (RE = rare earth) thick films [6], single crystals [7] and melt-texture bulks [8], an understanding of the melting behaviour of YBCO thin films is significant for both technological applications and a fundamental understanding of the melting mechanism. In this work we present a detailed comparison of the melting mode of YBCO thin films with different in-plane orientations. The mechanism was clarified on the grounds of interface energy.

2. Experimental details

The YBCO thin films were deposited on MgO single-crystalline substrate separately by magnetron sputtering and thermal co-evaporation. Both films are *c*-axis oriented. The *a–b* alignment of the films was tested by XRD pole figure (D8 Discover GADDS, Bruker AXS). The melting behaviour of the films was observed *in situ* through a high-temperature optical microscope (BX51M). Before observation, the system was calibrated using pure silver, whose melting point is 961 °C. Measured by a Pt/Rh thermocouple, the temperature of the sample was controlled within ±1 °C of the set value by a microcomputer. For convenience, we mark the film prepared by magnetron sputtering as film A, while the other film is film B. The thickness of film A is 330 nm, while the thickness of film B is 100 nm. The heating procedure, which started from room temperature, is shown in table 1. All observations were conducted in air. Based on the observed result, vertical dipping LPE experiments [9] were performed as another measurement of the thermal stability of the films. The temperature was within the range 995–1002 °C, which is lower than the T_p of Y123 (1010 °C).

3. Results and discussion

The melting behaviour of the two YBCO films showed great differences. Figures 1(a) and (b) represent the initial stage of melting of film A. As shown in figure 1(a), many needle-like

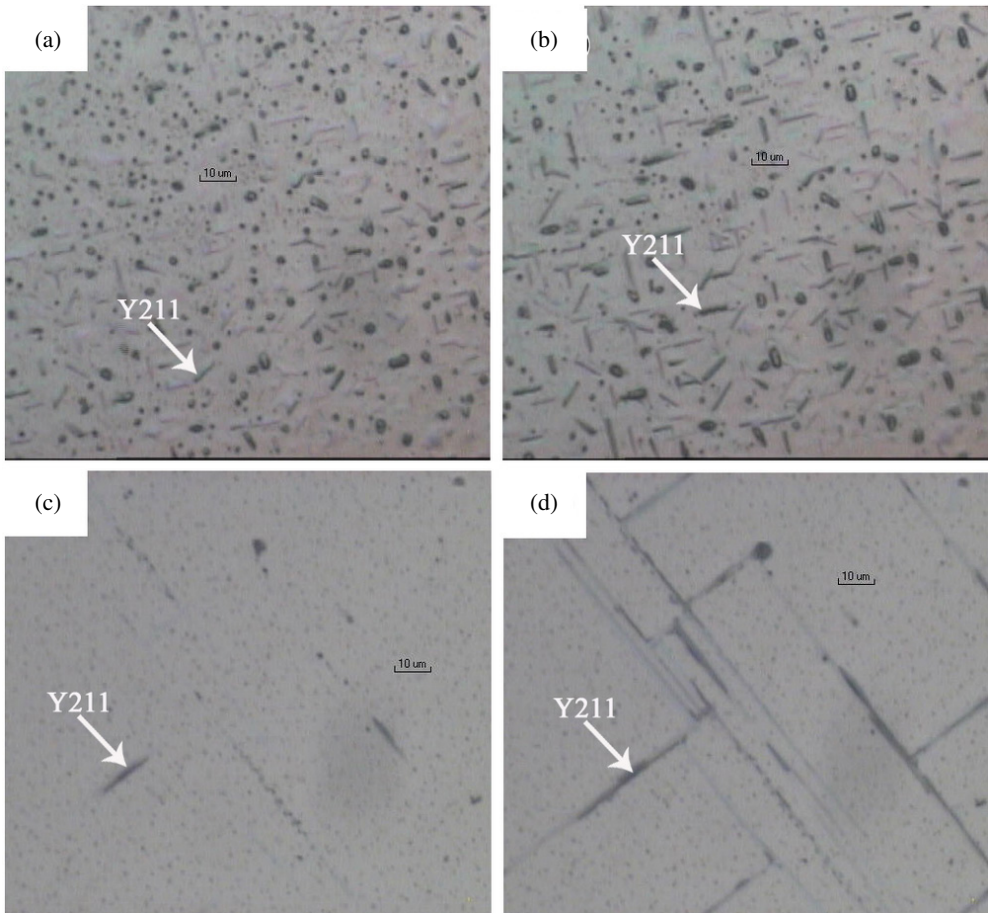

Figure 1. Optical micrographs showing the initial stage of melting of two YBCO thin films: (a) film A at 970 °C; (b) film A at 978 °C; (c) film B at 1032 °C; (d) film B at 1040 °C.

Y_2BaCuO_5 (Y211) crystals appeared under the surface of the film when the temperature reached 970 °C. The big black droplets were BCO melt. When the temperature reached 978 °C, more Y211 crystals appeared (figure 1(b)). Interestingly, the growth of Y211 in the *c*-axis was hardly identified, implying that the crystals almost grew over before they showed up on the surface of the film. There are four points to which one should pay attention. First, at the outset of melting, the surface of the film stayed uniform. No substrate was observed between the Y211 crystals and the Y123 film. Second, the number of Y211 crystals is large. Third, the grains with 0° (Y211⟨001⟩ ∥ MgO⟨100⟩) and 45° (Y211⟨001⟩ ∥ MgO⟨110⟩) orientations appeared simultaneously. Fourth, the melting began at a temperature 40 °C lower than the T_p of Y123.

For film B, firstly, Y211 crystals began to appear as several short dashed lines, which are illustrated by the small left-hand photograph in figure 1(c). Notice that the temperature was 1032 °C, higher than the melting point of Y123. Compared with film A, the amount of Y211 is small. Then a clear growth along the *c*-axis of Y211 was evident, while the Y211 phase gradually emerged as a solid straight line (1040 °C, figure 1(d)). Most Y211 crystals had a 45° orientation, which is known as the preferential growth orientation of Y211 on the MgO substrate [10].

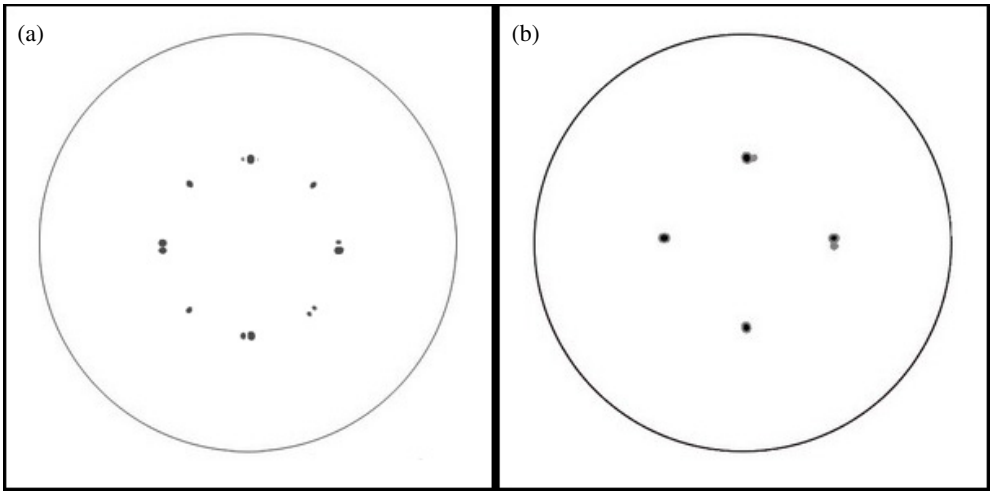

Figure 2. XRD pole figure of two YBCO thin films: (a) film A; (b) film B.

In order to clarify the mechanism of melting modes, some further characterization of the microstructure of the films is required. An XRD pole figure was carried out to detect the in-plane orientation of the film. Figure 2(a) was the pole figure of film A, which can be recognized as a mainly eightfold symmetry with some additional peaks. This pattern shows that both 0° (YBCO$\langle 100\rangle_{\text{film}} \parallel \text{MgO}\langle 100\rangle_{\text{substrate}}$) and 45° (YBCO$\langle 100\rangle_{\text{film}} \parallel \text{MgO}\langle 110\rangle_{\text{substrate}}$)123 grains exist. The poor in-plane alignment implies weak epitaxial confinement at the YBCO/MgO interface as a whole. In contrast, significant distinction was found in the pole figure of film B. Illustrated by figure 2(b), a fourfold symmetry indicates that only 0° orientation grains exist. This fine epitaxial relation exhibits a semi-coherent interface at the film/substrate interface.

From the viewpoint of interface energy, the different melting mode of the two films can be elucidated. For film A, the weak epitaxial interface implies the existence of additional defects and grain boundaries, which store large excess energy and constitute an extra driving force for the melting. As a result, the melting occurred simultaneously at the film/substrate interface at a relatively low temperature. The nucleation and growth of Y211 grains were also encouraged due to the high-energy interface. This is supported by the large number of Y211 grains and the appearance of grains with non-preferred orientation. The nuclei grew along the interface quickly and broke the entire bonding between the film and the substrate; as we observed, many Y211 appeared while the film surface stayed uniform. As for film B, the semi-coherent interface played a critical role in understanding the melting behaviour. It is well known that the energy of coherent and semi-coherent interfaces is significantly lower than that of noncoherent interfaces [11]. At the same time, the nucleation of melting requires a sufficiently large driving force. Owing to the combination of these two points, the primary signal of Y123 decomposition loomed at a temperature higher than the T_p of Y123. The small quantity of Y211 can be further proof of the adequately suppressed nucleation rate. Moreover, the semi-coherent interface forms a barrier against the growth of melt as well. When melt nuclei grew along the interface, breaking the strong bonding between film and substrate demands enough extra energy. So the growth of Y211 is slow enough to be captured by the naked human eye under optical microscopy. Unlike film A, in which 45° grains and 0° grains are present together,

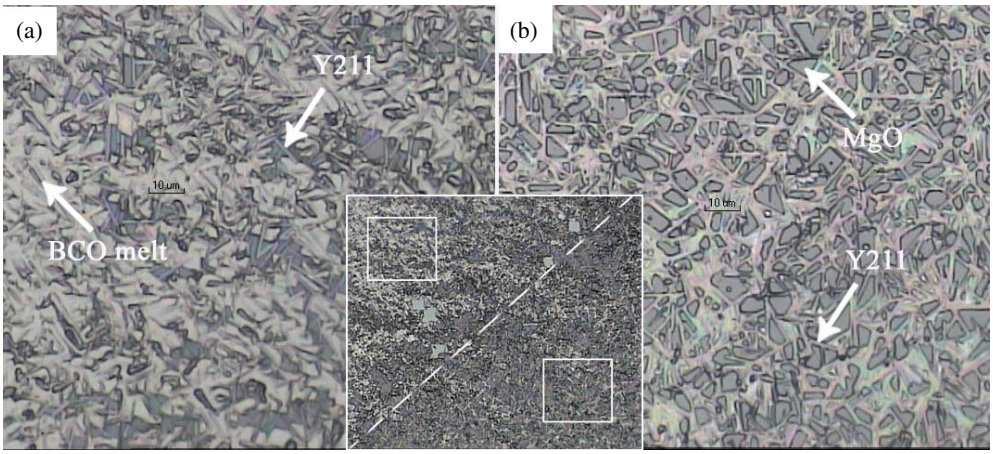

Figure 3. The dipping outcome of film A: the inset gives a general view of the boundary region, with the white dashed line marking out the dipped region on the upper-left corner and the undipped part on the opposite corner, while (a) is an enlarged image of the square area on the dipped side and (b) is an enlarged image of the square area on the undipped side.

45° grains occupied the majority of the Y211 population at the outset of melting in film B. On the grounds that the 45° orientation growth required the minimum energy supply, this selective growth gives one more demonstration of the suppression of melt growth. Regarding the first report of thin-film superheating by Zhang *et al* [5], only a small fraction of Pb layers was found to have semi-coherent Pb/Al interfaces. They suggested that the nucleation of melting could not be prevented and that the superheating was due to the suppression of melting growth. Combining their results with ours, it can be deduced that a fine epitaxial confinement restrains both the melting nucleation and growth, while a partial epitaxial interface only delays the melting growth. The suppression of melting nucleation is of vital importance in the respect that even partial melting may cause devices to malfunction. In short, poor in-plane alignment could be an excess energy source that encourages melting/decomposition at the interface (in our case, the Y123/MgO interface), while a fine alignment, with lowered interface energy, could be an obstacle against melting/decomposion.

To confirm our supposition, vertical dipping LPE experiments were performed. The temperature of the liquid, within the range 995–1002 °C as we mentioned before, was carefully chosen between the initial melting points of film A and that of film B. The inset of figure 3 gives a general view of film A after dipping, with a white dashed line marking out the dipped region on the upper-left corner and the undipped part on the opposite corner. Several Y123 grains with 0° orientation could be identified along the division line. Knowing that the Y123 grain could not grow directly on MgO substrate without a seed in LPE dipping, there must be some 0° oriented Y123 grains, which had an epitaxial relation with MgO, surviving and acting as seeds during dipping. This result confirmed the strengthened thermal stability of grains with epitaxial confinement. Figure 3(a) shows an enlarged image of the square area on the dipped side in the inset. Thick BCO flux covered a large part of the area. No Y123 grain was identified. Figure 3(b) corresponds to another square area on the undipped side, where a large amount of randomly oriented Y211 grains were slightly covered by BCO melt. In agreement with our HTOM observation, both sides of the film indicated a nearly complete decomposition of the film, even though the dipping temperature was lower than the T_p of Y123. As to film B, at such

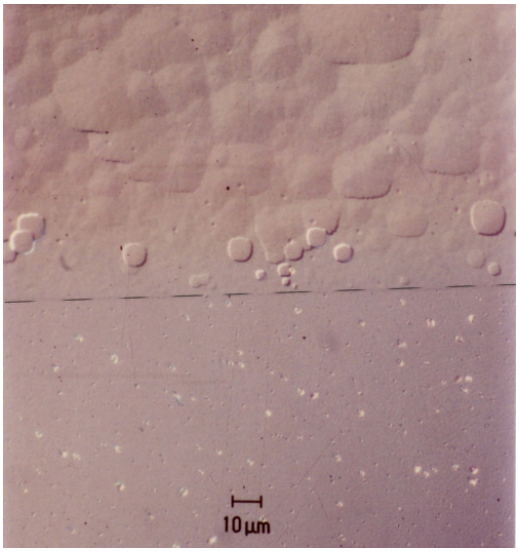

Figure 4. The dipping outcome of film B: the upper side is the area touched by liquid; the bottom side is the area untouched by liquid.

a relatively low temperature, the film would not decompose. The liquid-touched film acted as a seed film for the LPE growth of YBCO thick film, while the untouched area remained unchanged. Illustrated in figure 4, divided by a black dashed line, an LPE thick film covered the whole dipped region on the top side, while the bottom side, where the liquid did not touch, stayed the same as it was before dipping. The strong thermal stability of film B was confirmed.

4. Conclusions

In summary, an obvious deviation of the melting mode between YBCO thin films was found in both HTOM observation and LPE experiments. Based on the interface structures detected by XRD pole figures, the melting mechanism was clarified. A fine epitaxial confinement results in the suppression of melting nucleation and growth. In contrast, poor alignement of the thin film leads to the simultaneous nucleation and unimpeded growth of melt nuclei.

Acknowledgments

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