INVESTIGATION OF EPITAXIAL NIOBIUM THIN FILMS GROWN ON DIFFERENT SURFACES SUITABLE FOR SRF CAVITIES*

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Abstract

Superconducting radio frequency (SRF) technology used in linear accelerators is based on bulk Nb cavities that have high costs and are approaching the maximum field gradients they can withstand [1]. Thus, development of a suitable alternative to bulk Nb is needed. Several attempts with varying degrees of success have been made to implement Nb-coated Cu cavities since the thermal conductivity of Cu is better than bulk Nb [2]. Our studies show that the transport properties of Nb, in particular the residual resistance ratio (RRR), are better when Nb is epitaxially grown on crystalline ceramics (i.e. MgO and Al_2O_3) compared to Cu templates. Since grain boundaries are one of the main obstacles to superconducting transport, we show how the increased number of crystallographic domains that can occur during epitaxial Nb growth onto Cu surfaces leading to higher density of grain boundaries can explain these results. We propose a route to improved performance while keeping thermal efficiency advantages by using epitaxial seed-layers on Cu templates that can decrease grain boundary density in the final Nb film. We will show our correlated studies of microstructure and surface morphology and the resulting transport/susceptibility properties illustrating possible mechanisms to improve cavity performance of such films.

EPITAXIAL NIOBIUM FILMS

Film Deposition

Epitaxial Nb films have been prepared by DC magnetron sputtering at 1 mTorr on various surfaces including MgO (100), Al_2O_3 (11-20), Cu (100), and MgO reactively sputtered onto Cu (100). The ceramic MgO and Al_2O_3 substrates used were acquired commercially while the Cu surface was prepared by depositing fresh Cu layers onto Si (100) [3] in UHV in order to avoid native oxides as well as surface treatments that might complicate our growth studies. The thickness of the films studied ranged from 500-600 nm. On both MgO and Al_2O_3 substrates, the growth temperature was held at 600 °C which was found to lead to optimized films, while the Cu/Si substrate temperature was constrained below 175 °C in order to prevent silicide formation at the Cu/Si interface. The micro-structure of the films was studied *in-situ* with reflection high-energy electron diffraction (RHEED) and the surface morphology of the films was examined *ex-situ* with atomic force microscopy (AFM) and associated software [4]. In order to simplify the discussion, the samples that were investigated here have been designated as sample A-E and their growth conditions are listed in Table 1.

Table 1: Summary of Sample Parameters

Name	Substrate	Nb Orientation	Nb Thickness	Nb Growth Temp
A	MgO (100)	(100)	500 nm	600 °C
B	MgO (100)	(110)	600 nm	600 °C
C	500 nm Cu (100) / Si (100)	(110)	500 nm	150 °C
D	1 nm MgO/ Cu (100)/ Si (100)	Polycrystalline	500 nm	150 °C
E	Al_20_3 (11-20)	(110)	600 nm	600 °C

Microstructure and Surface Morphology

The epitaxy of the deposited Nb film is highly dependent on the choice of substrate. In the case of an MgO (100) surface, Nb films will either grow (100) oriented with only one possible grain structure, Nb(100)[011]||MgO(100)[001], or (110) oriented with two possible grain orientations, Nb(110)[-1-10]||MgO(100)[001] and Nb(110)[001]||MgO(100)[001] [5]. In the case of Nb growth on Cu (100), there are four possible grain orientations that can form such that Nb(100)[111]||Cu(100)||[110] [6]. A visual depiction of the possible orientations of Nb on MgO (100) and Cu (100) is shown in Figure 1. Nb also grows (110) oriented on Al_2O_3 (11-20) [7].

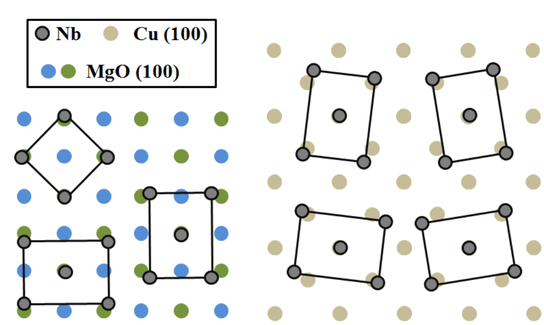

Figure 1: Overlays of a relaxed Nb lattices on MgO (100) and Cu (100).

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The RHEED patterns associated with our films agree very well with the predicted epitaxy as shown in Figure 2.

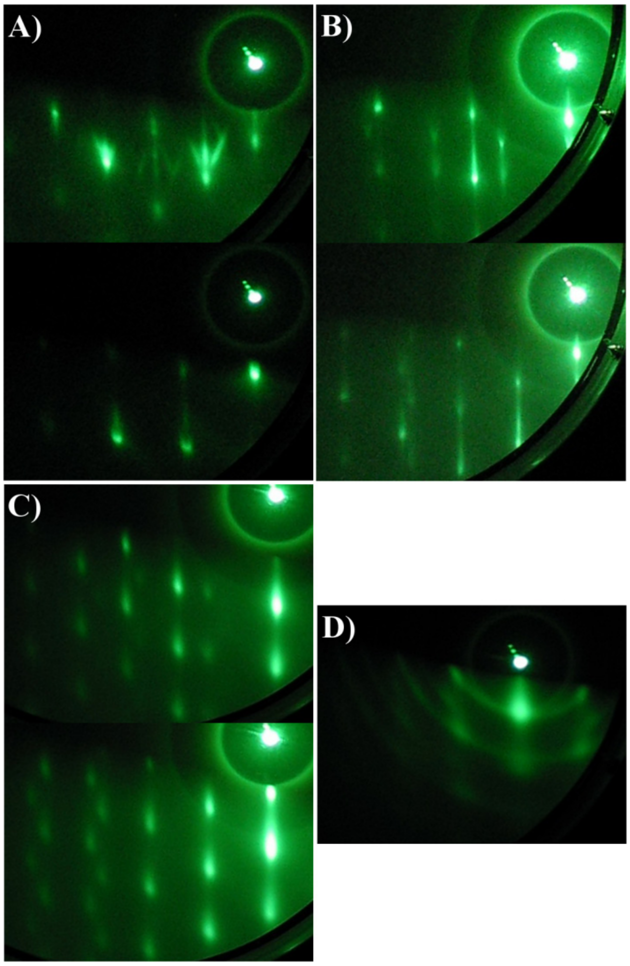

Figure 2: A) Sample A Nb pattern along the MgO[100] (top) and [110] (bottom) directions. B) Sample B Nb pattern MgO[100] (top) and [110] (bottom) directions. C) Sample C Nb pattern along the Cu [100] (top) and Cu [110] (bottom) directions. D) Sample D shows a highly textured polycrystalline surface. Note: Sample E is not shown here.

We note that very sharp streaks in Figure 2 (A) and (B) are indicative of high crystalline quality, with large grain size. Faceting is evident on Sample A indicated by the appearance of chevron features in Figure 2 (A). The broader streaks noticed in Figure 2 (C) indicate a material with smaller grains. Figure 2 (B)(top) and (C)(top) show a superposition of two different patterns with separation distances with a √2 ratio, which agrees with the discussed epitaxy corresponding to equivalent uniaxial grains that are oriented 90° with respect to each other. Figure 2 (B)(top) has inter-streak spacings that correspond to the other possible domains on Cu (100) that are not perpendicular. The patterns found in Figure 2 (B)(bottom) and (C)(bottom) are contributions from the Nb(-111) and (-112) planes [6]. The superposition of streaks and rings in Figure 2 (D) indicates a polycrystalline surface with a high degree of texture.

We note that the nature of the film epitaxy has a strong effect on the resulting surface morphology as shown in Figure 3. Figure 3 (A) shows regular distribution of 4-fold symmetric features consistent with (100) single domain found in Nb(100)/MgO(100) growth. In the case of Sample B, there are two possible perpendicular domains with uniaxial anisotropy leading to perpendicular uniaxial surface features as shown in Figure 3(B). Figure 3 (C) shows perpendicular features as well which also agrees with the two sets of perpendicular domains found in the Nb(110)/ Cu(100) system shown in Figure 1. The surface features in Figure 3 (D) are more randomly oriented, agreeing with the polycrystalline RHEED pattern.

Because SRF properties are constrained to the surface in accelerator cavities, understanding how the surface morphology affects the superconducting transport is crucial. We discuss this next.

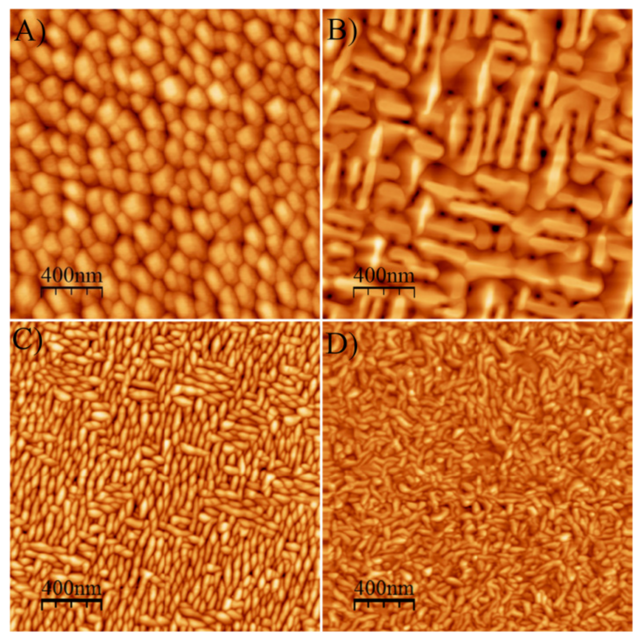

Figure 3: AFM scans for (A) Sample A, (B) Sample B, (C) Sample C, and (D) Sample D. Note: Sample E is not shown here.

TRANSPORT AND SUPERCONDUCTING PROPERTIES

Comparison of RRR

A common measure of transport merit in Nb thin film samples is their RRR value. Typically, a RRR value larger than 250 is desired for Nb sheets to be used in cavity fabrication [1]. Thin film RRR values are typically lower than bulk values due to a higher number of structural defects resulting from deposition processes as well as the effect of interfacial scattering. We note here that it has been shown that RRR values in thin films are highly dependent on the film thickness and typically saturate above a few microns [8].

The RRR values of Samples A-E are listed in Table 2. Because the films are similar in thickness, although not suitable for cavities, their RRR values can be compared to each other to assess improvement venues for the growth. We note a direct correlation between the decrease in number of possible domains and the increase in RRR value in many of these films. Thus, we interpret this correlation to the fact that grain boundaries are one of the main inhibiting factors in superconducting transport. It is important to mention that RRR values on films deposited on Cu are also affected by the transport properties of Cu as well.

Table 2: Comparison of RRR values

Sample	RRR	Possible Domains
A	165.5	1
B	46.5	2
C	19	4
D	8.7	Polycrystalline
E	96	2

Critical Temperature and Critical Fields

The superconducting properties, critical temperature (T_C) and critical fields (H_{C1} and H_{C2}), of the films were also probed using SQUID magnetometry. The transition from the superconducting to non-superconducting phase of the films, as shown in Figure 4, generally occurred around the bulk T_C value of 9.2 K. As discussed earlier, thin films typically have a higher number of defects which can inhibit transport properties. This increase in defects makes it more difficult for a material to enter the superconducting phase and effectively lowers T_C values. An example of this is seen for Sample A whose T_C is closer to 9 K.

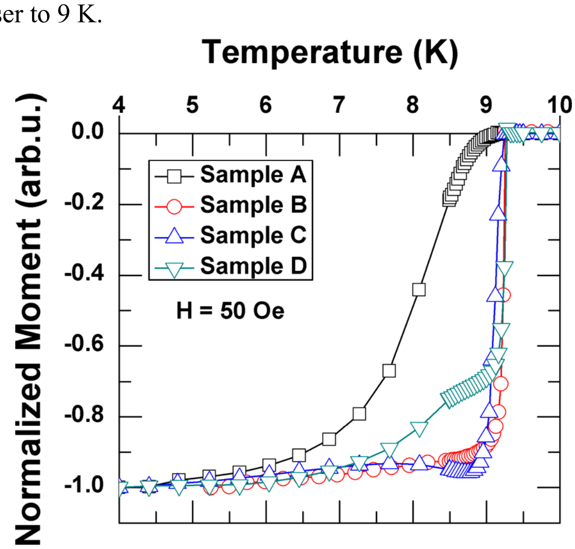

Figure 4: Critical Temperature transitions.

In general, as the grain boundary density increased, the critical fields, H_{C1} and H_{C2}, increased. Even though it is desirable to have cavities that can withstand greater magnetic fields, the detrimental effects of grain boundaries on transport properties would cause the overall performance of the cavity to suffer.

DISCUSSION AND OUTLOOK

We have shown that decreasing the grain boundary density in Nb thin films improves transport properties such as RRR. In order to achieve Nb coated Cu cavities with optimal performance, it may be necessary to overcome the multiple growth domains of Nb on Cu (four domains on Cu (100) and six domains on Cu (111)). To overcome these domains, we have explored several seed layer materials to place between the Cu surface and the Nb film. We have been able to grow epitaxial multilayered structures with promising seed layers such as MgO, Pd, and Au. Despite achieving epitaxial growth, the process of minimizing grain boundary density is still being optimized.

In addition to increasing the performance of cavities by incorporating materials with better thermal properties, such as Cu, it has also been proposed to use superconducting-insulating-superconducting (SIS) structures on top of the Nb surface [9]. This SIS structure involves superconducting materials that can shield the Nb from higher magnetic fields because they have higher H_{C1} values. As a starting point, we have successfully grown and characterized an epitaxial multilayer of Nb/MgO/Nb on an MgO (100) substrate. Once the performance of this structure is understood, the top Nb layer will be replaced with a more desirable superconductor (with a higher H_{C1} value), such as NbN, Nb_3Sn, or MgB_2. Other insulators may also be investigated to optimize structural and transport properties.

Ultimately, these two approaches to improving cavity performance will be combined to have the SIS structure on a suitable Nb film on a Cu template. This combination will increase the thermal efficiency of the cavity while allowing the accelerating gradient to be increased as well.

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