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Coated conductors containing grains with big aspect ratios

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Abstract. It is shown that the critical currents of high-T_c superconducting tapes fabricated by the coated conductor technologies are enhanced considerably if grain arrangements with large effective grain boundary areas are used. Increasing the aspect ratios of the grains reduces the deleterious effects of the grain boundaries. A practical road to competitive high-T_c cables is proposed.

Cables that are superconducting at 77 K require the use of polycrystalline high-T_c-superconductors [1] with large critical currents. For materials with sufficient pinning, such as $YBa_2Cu_3O_{7-\delta}$ [2], three strategies have been found to achieve this goal. The first is to enhance the *critical current density* of the grain boundaries. This can be done by aligning the grains along all three major axes to within few degrees [3]. This approach is based on the fact that the grain boundary critical current density is an exponential function of the misorientation angle [4], dropping by three to four orders of magnitude as the misorientation angle is increased from 0° to 45°. Second, for a given misorientation angle, the grain boundary critical current density is enhanced by appropriate doping [5, 6]. The third strategy consists in maximizing the effective *grain boundary area* by optimizing the arrangement and the shape of the grains, as illustrated in Fig. 1. In the simplest case, this can be achieved by utilizing grains with large aspect ratios [7, 8].

The most promising candidates for economically competitive cables are tapes fabricated by coated conductor technologies, such as ion beam-assisted deposition (IBAD) [9], rolling-assisted biaxially-textured substrates (RABiTS) [10, 11], and inclined-substrate deposition (ISD) [12, 13]. For practical applications, the coated conductor technologies are superior to the competing powder in tube technology which is based on Bi-based high-T_c superconductors embedded in silver tubes, because the material costs of coated conductors are decisively smaller and the $ReBa_2Cu_3O_{7-\delta}$ superconductors, where Re is Y or a rare earth, and they offer the potential of operation at 77 K in large magnetic fields. The best coated conductors fabricated at present support critical current densities exceeding $10^6\,\mathrm{A/cm^2}$ over meter lengths. Taking the substrate thickness and thereby the whole cross-section of the tape into account, these current

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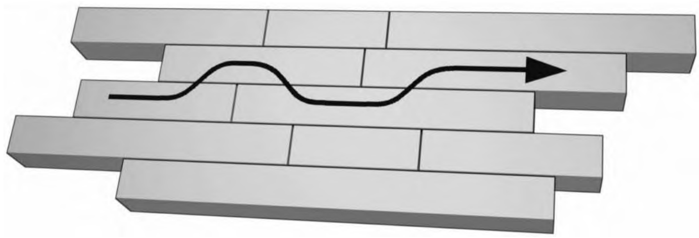

Fig. 1 Sketch of a brick-wall like arrangement of grains in a coated conductor. The arrow illustrates a possible path for the supercurrent. The current traverses grain boundaries with large areas

densities correspond to engineering critical current densities of several $10^4\,\mathrm{A/cm^2}$. These values are achieved by aligning the grains along all axes with a spread of misorientation angles smaller than $10\,^\circ$. Because the corresponding grain alignment processes are slow and costly, strategies are urgently sought to enhance the critical current density of such tapes for a given misorientation spread. The solution of this problem would provide the key to commercially viable large scale applications of high-T_c superconductors.

Applying the concepts conceived in [7] to coated conductors, we suggest to enhance their critical currents I_c by using grains with large aspect ratios to optimize the effective grain boundary area (see Fig. 1). According to the model calculations described below, an increase of the average grain aspect ratio causes a monotonous, strong increase of I_c, as well as a reduction of the sensitivity of I_c to the average grain boundary angle.

The calculations performed to analyze the critical current of a given grain boundary network were based on a modified version of the algorithm developed by Holzapfel *et al.*, as described in detail in [14]. This algorithm has been designed to analyze the critical currents of grain boundary networks in coated conductors. The procedure considers two-dimensional grain networks characterized by a given spread of grain orientations. In such a network the algorithm searches for the cross-section that limits the critical current, and then calculates the critical current of this cross-section. Because for the grain misorientations of interest the grain boundaries do not act as Josephson junctions, and all phase effects are negligible. As shown in [14], the results of such calculations agree well with transport measurements of I_c. For our work, the algorithm was optimized for speed, so that several thousand networks, each containing $10^5 - 10^6$ grains, could be calculated on a personal computer. This optimization was achieved by accelerating the search for the limiting cross-section, storing information gained in the individual search routines.

To analyze the effect of the enhancement of the effective grain boundary area on I_c, two-dimensional arrays of N grains arranged in brickwall-type structures were considered (see Fig. 2 and Fig. 3). In these structures to each grain an in-plane orientation α_i was assigned (see Fig. 2). Whereas the same width w was selected for all grains, the length l_i of each grain was randomly chosen, following a Gaussian distribution with a full width at half maximum (FWHM) of $l/5$ centered around the average length l, clipped to zero below $w/2$ and above 250 w. The average aspect ratio of the grains is then given by $N^{-1}\sum l_i/w$. As the critical current of the network is also affected by the intragranular critical current density $J_\mathrm{c}^\mathrm{grain}$, each

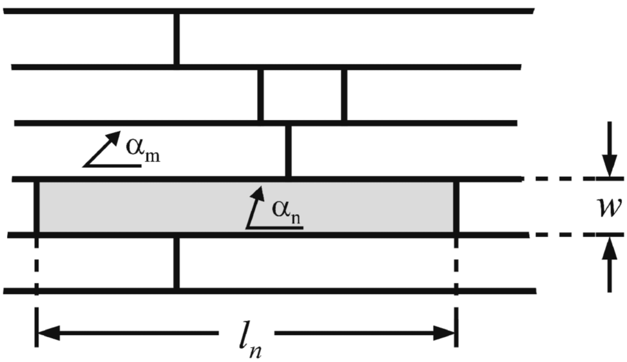

Fig. 2 Illustration of the grain arrangement considered in the calculations

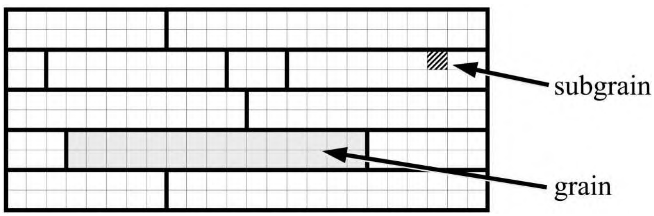

Fig. 3 Sketch of the grain and subgrain arrangement in a small array consisting of 24 * 10 subgrains. The thick lines represent the grain boundaries. The thin lines show the boundaries between the subgrains

grain was split into two rows of square subgrains (see Fig. 3) and the critical current density of the boundaries between the subgrains was set to equal $J_{\mathrm{c}}^{\mathrm{grain}}$.

The angles α_i were also randomly chosen, again following a Gaussian distribution, this time centered at 0 ° with a FWHM-spread σ. Values of α_i exceeding 45 ° were clipped.

The grain arrangements and the Gaussian distributions were selected to provide clear and simple rules for the design of the model systems. These systems are presented as first examples for practical conductors with more complicated designs. As will be obvious, the conclusions of our work are not affected by the particular choice of the model systems used for the calculations.

In case self field effects are negligible, the critical current of the grain boundary between two grains, n and m, is well approximated by the product of the boundary area and its critical current density $J_{\mathrm{c}}^{n,m}$. To calculate the critical current density, an exponential dependence on the misorientation angle $|\alpha_n - \alpha_m|$ was used [4]

$$J_{\mathrm{c}}^{n,m} = J_{\mathrm{c}}^{\mathrm{grain}} \cdot \exp(-\frac{|\alpha_n - \alpha_m|}{\beta}). \tag{1}$$

Here $J_{\mathrm{c}}^{\mathrm{grain}}$ was set to $5 \cdot 10^6 \mathrm{A/cm^2}$ and β to 5.3 °, values typical for coated conductors operated at 77 K. With this, the influence of the grain aspect ratio on the critical current of the network was analyzed. For a series of average aspect ratios and grain orientation distributions the critical current densities of networks 200 subgrains wide and 1,000 subgrains long were calculated. Depending on the grains' average aspect ratios these networks consisted of about 500 to 50,000 grains. For each set of parameters the critical current densities of at least 20 different networks have been determined and the resulting critical current densities averaged. Fig. 4 shows the resulting critical current densities. The error bars display the standard deviation of the calculated currents as determined from the averaging process.

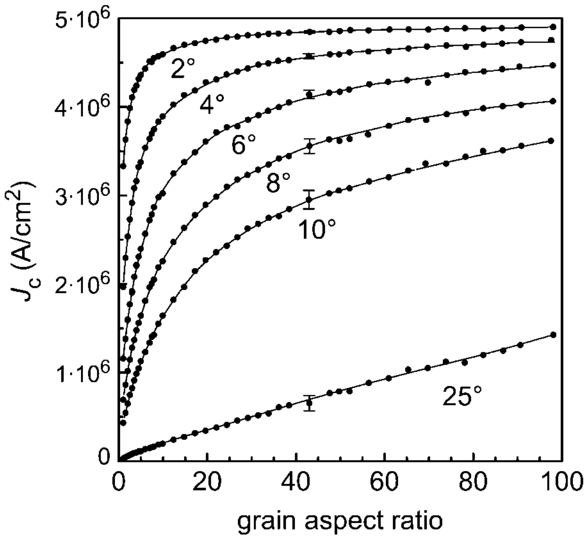

Fig. 4 Plot of the critical current density J_c as a function of the average grain aspect ratio, calculated for various grain alignment spreads σ. The data have been obtained in calculations on grain networks consisting of 1000 * 200 subgrains. Each datapoint reflects an average of at least 20 calculations. The lines are guides to the eye

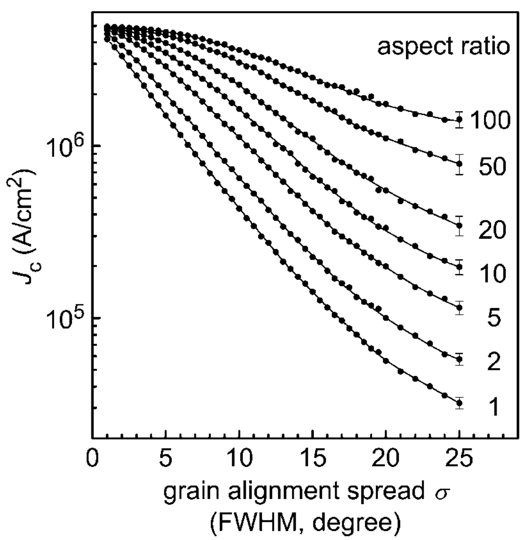

Fig. 5 Plot of the critical current density J_c as a function of the grain alignment spread σ, calculated for various average grain aspect ratios. The data have been obtained in calculations on grain networks consisting of 1000 * 200 subgrains. Each datapoint reflects an average of at least 20 calculations. The lines are guides to the eye

As shown by the figure, the critical current density of the network rises strongly and monotonously with increasing aspect ratio of the grains. The gradient is largest at small aspect ratios, which is attributed to the relatively small current densities of these networks, which are barely affected by J_c^{grain}. For small misorientation angles and large aspect ratios the current densities saturate at J_c^{grain}. The calculated J_c enhancements are impressive. For example, for grain misorientations resulting from an alignment spread of $10\,^\circ$, the current densities are enhanced from $4.4 \cdot 10^5\,\mathrm{A/cm^2}$ to $1.6 \cdot 10^6\,\mathrm{A/cm^2}$ if the average aspect ratio is increased from 1 to 10.

Further, the dependence of the critical current on the spread σ of the grain orientations was analyzed, considering various average aspect ratios. The results of these calculations are shown in Fig. 5. As expected, for small angular spreads the critical current densities of the networks equal the intragrain critical current density, independent of the aspect ratios. Surprisingly, in networks consisting of grains with large aspect ratios, the well known exponential drop of J_c with misorientation is modified and damped. Approaching the intragranular current density, coated conductors with a grain alignment as large as 10° and grain aspect ratios of 50 have the same critical current density as standard coated conductors (aspect ratio 1) with a misalignment of only 2°. Networks with aspect ratios ~ 100 support critical current densities exceeding $10^6\,\mathrm{A/cm^2}$ for grain alignment spreads as large as $\sigma = 25^\circ$.

Although the calculations presented consider particularly simple, mathematically accessible tape structures and neglect self field and second order effects, they clearly show the usefulness of optimizing the grain structure in the coated conductor technologies, in particular the use of grains with large aspect ratios.

The realization of coated conductors with big aspect ratios we consider to be technologically straightforward. The IBAD or ISD processes may be modified so that grains with large aspect ratios are nucleated, for example, by taking advantage of anisotropic diffusion during grain nucleation and growth. The RABiTS architecture is particularly suited for the implementation of grains with big aspect ratios. For example, metallic tapes with standard RABiTS texture, consisting of Ni-alloys or steel, may be rolled and annealed in mass production processes to contain long grains which are aligned parallel to the length of the tape. Standard RABiTS buffer layer and superconductor epitaxy, performed by cheap deposition processes under development, will reproduce this grain structure in the $ReBa_2Cu_3O_{7-\delta}$-based superconductor, yielding at competitive costs high-T_c tapes with very large critical currents.

In summary, suggesting a solution to the grain boundary problem, we propose a practical road to competitive high-T_c cables: fabricating doped coated conductors containing grains with big aspect ratios.

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Note added in proof:

As twinning was not considered, Eq. 1 was unintentionally applied for angles $|\alpha_n - \alpha_m| > 45°$, which results in a minor ($\approx 10\%$) reduction of the apparent critical current density of networks with very large σ-values.