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Prediction of decoupling in high-temperature superconductors

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The variation of magnetization with field in high-temperature superconductors was calculated by extending the spin-glass model of Ebner and Stroud [C. Ebner and D. Stroud, Phys. Rev. B 31, 165 (1985)] to incorporate domains inside the grains. Two coupling energies were used, one between domains in the same grain, and a field-dependent coupling energy between domains in different grains. The field dependence was assumed to be the same as the field dependence of critical current density. This model reproduces the experimentally observed decoupling of superconductors at low fields.

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I. INTRODUCTION

The 90-K superconductors can be modeled as a granular superconductor with Josephson junctions between the links.[1] Monte Carlo simulations of this model[2] qualitatively reproduce many of the features of the new materials. However, at very low magnetic field, there is an anomalous feature in the experimental magnetization versus field plot[3,4] that the model cannot reproduce. The focus of this Rapid Communication is modification of the model to predict this behavior.

II. THE EBNER AND STROUD MODEL

The Hamiltonian for a system of granular superconductors[1,5] is

$$H=-\sum_{\langle ij\rangle} J_{ij}\cos(\theta_i-\theta_j-a_{ij})\,, \tag{1}$$

where the ith grain is located at $\mathbf{x}_i$ and has a complex energy gap

$$\psi_i=\Delta_i e^{i\theta_i}\,, \tag{2}$$

where θ_i is the phase angle of the coherent electrons in grain i. The coupling energy J_{ij} is the energy between adjacent grains i,j. The a_{ij} are the phase factors and are given by

$$a_{ij}=\frac{2\pi}{\phi_0}\int_i^j \mathbf{A}\cdot d\mathbf{l}=\frac{2\pi}{\phi_0}H\frac{x_i+x_j}{2}(y_j-y_i)\,, \tag{3}$$

where x_i, y_i are the actual coordinates of the ith grain and ϕ_0 is the elementary flux quantum. The following[2] locations are chosen randomly within circles of radius $0.2a$ centered on lattice sites where a is the spacing between the sites.

It has been suggested[2] that the junctions represent connections between intragranular regions of coherent phase (domains) rather than between grains. There is evidence both in favor[6] and against[7] this idea. In either case, the model does not capture the behavior of an individual domain (or grain), which would have screening currents. Rather, the domains are taken as points. Josephson currents circulate from domain to domain coupled into loops.

Simulations of the above model with J_{ij} held constant for nearest neighbors and zero otherwise gives qualitative agreement with experimental magnetization versus field data.[2,8] In this work 100 spins were used. The system was cooled from a dimensionless temperature of $kT/J=1.5$ to a temperature of 0.45 in 17 steps. All simulations were done at constant field. At each temperature 10000 Monte Carlo passes were executed, the first 5000 being used to equilibrate the system. Data was collected over the second 5000 steps. Previous simulations[2] were continued to much lower temperatures and so needed much longer runs. The adequacy of the length of the run used here was tested by doubling the number of passes, by reheating the system, and by checking that the autocorrelation function

$$C(t,t_0)=\frac{1}{N}\sum_{i=1}^{N}\mathbf{s}_i(t)\cdot\mathbf{s}_i(t_0)=\frac{1}{N}\sum_{i=1}^{N}\cos[\theta_i(t)-\theta_i(t_0)] \tag{4}$$

averaged over fifty initial configurations went to zero.

The simulations predict that magnetization (dimensionless)

$$\frac{M\phi_0}{NJa^2}=2\pi\sum_{\langle ij\rangle}\left[\frac{x_i+x_j}{2}\right](y_j-y_i)\sin(\theta_i-\theta_j-a_{ij}) \tag{5}$$

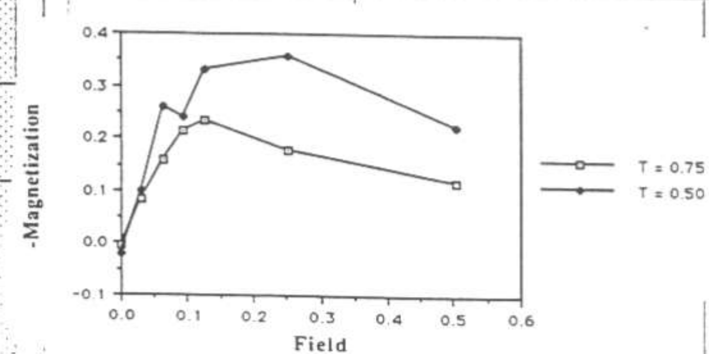

FIG. 1. Magnetization per spin ($M\phi_0/NJa^2$) vs dimensionless field ($2\pi\mu_0 Ha^2/\phi_0$) at two temperatures. No averaging over different runs has been done.

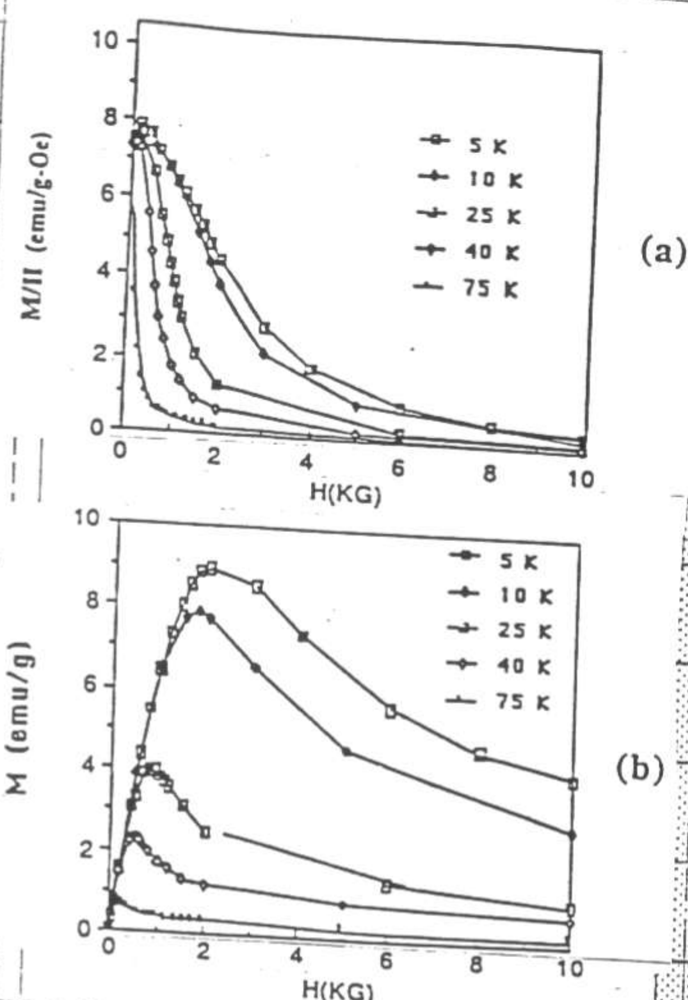

FIG. 2. Magnetization vs field at a range of temperatures for polycrystalline $YBa_2Cu_3O_{7-x}$. [Reproduced from McHenry *et al.* (Ref. 3). Note that the vertical axis should be labeled M (emu/g).]

should decrease with field, reach a minimum and then increase again. The lower the temperature the more negative the minimum in the magnetization versus field plot should be (Fig. 1). This is largely what is seen experimentally (Fig. 2). However, there is an anomalous feature at very low magnetic fields (Fig. 3) that the above model does not predict.

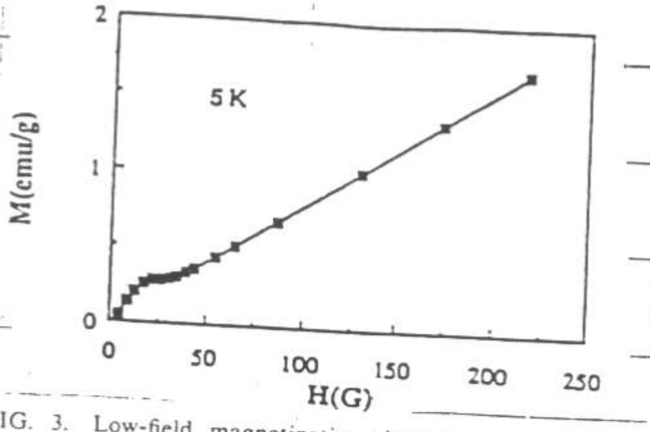

FIG. 3. Low-field magnetization data for polycrystalline $YBa_2Cu_3O_{7-x}$ [reproduced from McHenry *et al.* (Ref. 3)].

III. EXPLANATION OF THE LOW-FIELD MAGNETIZATION BEHAVIOR

The interpretation of the low-field data is that grains decouple at low fields. At very low field a polycrystalline material behaves as a bulk superconductor with almost complete flux expulsion. As the field is increased, the grains decouple[3] and the material behaves as a collection of almost independent grains. The magnetization falls initially because flux is excluded from a smaller volume but then increases because larger currents circulate to screen the whole sample.

Reproducing the low-field magnetization behavior requires a model for currents inside grains. We assume that there are superconducting domains inside the grains. The model represents currents between domains in the same grain as well as currents between domains in different grains (intergranular currents). The coupling energy between domains in the same grain is assumed to be unaffected by field at the low fields considered here, whereas the coupling energy between domains in different grains is field dependent.

A second feature in the magnetization versus field plot corresponding to the penetration of the field between domains is unlikely to be observed experimentally because the decoupling of the grains is smeared out over a range of fields and the decoupling of the domains represents an additional smearing.

IV. FIELD DEPENDENCE OF THE COUPLING ENERGY

The expression for the maximum current flowing from one grain to the next is given by

$$I_{ij}^{c}=\frac{J_{ij}}{\phi_0}. \qquad (6)$$

The behavior of the coupling energies as a function of field can thus be taken from experimental data for the field dependence of the critical current density.

The critical current density falls by an order of magnitude in fields as small as 20 Oe and then levels off to a plateau.[9] At much higher fields the current density again starts to fall. The behavior, until the plateau region is reached, is captured by averaging the equations for the field dependence of the critical current of a Josephson junction over an assumed distribution of junction lengths and orientations.[10] However, to capture the plateau region[9] the coupling energy is taken to be independent of field once it falls to a value of 0.15 of the zero field value (see Table I).

TABLE I. Field dependence of the coupling energy.

$\frac{H}{H_0}$	0.00	0.25	0.50	0.75	1.00	1.60	2.00
$\frac{J(H)}{J(0)}$	1.00	0.90	0.67	0.45	0.32	0.15	0.15

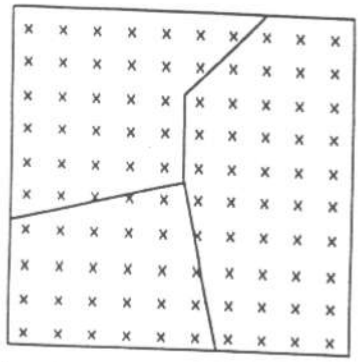

FIG. 4. Division of 100 spins into three grains. In the simulations the locations of the spins were randomly displaced a distance of 0.2 times the lattice spacing from the sites of a square array.

V. SIMULATION OF SYSTEMS WITH NONUNIFORM COUPLING ENERGY

It has been suggested[3] that the domains are between one 50th and one 500th the size of the grain. Others[11] infer that the domains are on a scale of less than one tenth the grain size. In the simulations the system of 100 spins (domains) was divided into three grains, giving domain sizes that are approximately one 30th the size of a grain. Figure 4 shows how the spins are divided into grains.

Simulation of many grains would reduce the importance of boundary effects but, as no new phenomena are introduced by the presence of additional grains, qualitative results are expected to be similar to be independent of system size.

Simulations using the above division of domains in grains, and incorporating Table I for the field dependence of the coupling energy between domains in different grains, gives a magnetization versus field plot shown as the lower curve in Fig. 5. The upper curve corresponds to simulations where all coupling energies are constant and independent of field (which corresponds to earlier simulations[2]). The field at which the maximum due to decoupling occurs is governed by the choice of H_0, which was taken to be 0.06 in Fig. 5. This value was chosen to ensure that the local maximum would not be swamped by noise in the data. Both graphs are a result of averaging over four independent runs, giving an accuracy of about $\pm 15\%$ in the data.

The shape of the lower curve in Fig. 5 is independent of the specific choices for the ratio of coupling energies and the number of domains per grain. Increasing the number of domains decreases the magnetization by increasing the number of loops that couple domains in different grains. Similarly decreasing the coupling energy between domains in different grains also depresses the magnetization.

The magnetization is also reduced in a more subtle fashion. In the limit where the coupling energy between grains is zero, spins on the boundary of the grains have three neighbors as opposed to four. The larger the number of neighbors, the larger the number of loops with which a given spin is associated and the greater the degree

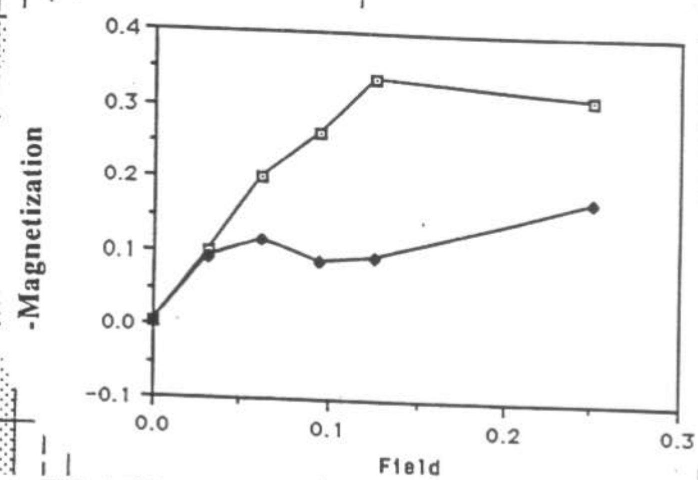

FIG. 5. Magnetization vs field for a system of 100 spins with three domains. In the lower curve, the coupling energy between domains in different grains is field dependent. In the upper curve the coupling energy is always unity. Both curves are a result of averaging four independent runs. The dimensionless temperature is 0.5.

of frustration. As the number of constraints is reduced, the argument of the cosine function in the Hamiltonian decreases and hence the magnetization decreases.

If all coupling energies had the field dependence of Table I, the ratio of slopes at fields smaller and greater than H_0 would be dictated by the ratio of the critical currents, and hence the coupling energy, on each side of the decoupling field (e.g., the ratio of slopes would be 0.15 from Table I). In experimental data the slope after the local maximum in the plot of negative magnetization versus field is smaller than but comparable to the initial slope. Consequently the experimental observations cannot be explained by Josephson behavior alone but rather require a modified model such as proposed here.

VI. CONCLUSIONS

The partial collapse of coupling energy of Josephson junctions located at grain boundaries was incorporated into two-dimensional spin-glass simulations. The results agree qualitatively with low-field experimental data for bulk polycrystalline materials. We expect that the same phenomenon should also occur for thin films. The simulations show that domains inside grains are consistent with experimental observations. However, the data can also be explained (but not modeled) without recourse to domains inside grains.

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