Growth of a vortex polycrystal in type II superconductors

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We discuss the formation of a vortex polycrystal in type II superconductors from the competition between pinning and elastic forces. We compute the elastic energy of a deformed grain boundary, that is strongly non-local, and obtain the depinning stress for weak and strong pinning. Our estimates for the grain size dependence on the magnetic field strength are in good agreement with previous experiments on NbMo. Finally, we discuss the effect of thermal noise on grain growth.

Understanding the phase diagram of high temperature superconductors is still a formidable challenge of modern condensed matter physics. Typically high $T_c$ materials behave in a magnetic field as type II superconductors, with further complications due to the broader phase space — in terms of temperature $T$ and field $H$ — in comparison to conventional superconductors. Raising the temperature, the Abrikosov vortex lattice melts into a liquid, while quenched disorder leads to more complex phases such as the vortex glass or the Bose glass. The natural question posed to the theorist is to explain the occurrence of the various vortex phases, linking the experimentally observed behavior with the material microstructure.

The Bitter decoration technique provides a powerful method to investigate the geometrical and topological properties of vortex matter by direct imaging of the vortices. Its application to conventional superconductors provided the first direct evidence of the vortex lattice predicted by Abrikosov. The lattice structure is often observed to coexist with topological defects, such as isolated dislocations, dislocation dipoles and grain boundaries. These last extended defects are the signature of a vortex polycrystal with crystalline grains of different orientations. Vortex polycrystals have been observed, after field cooling, in various superconducting materials such as NbMo, NbS$_2$, BSSCO, and YBCO. The grain size is typically found to grow with applied magnetic field. Moreover, two-sided decoration experiments show that the grain boundaries thread the sample from top to bottom, i.e., one observes a columnar grain structure. Despite the wealth of experimental observations, there is no detailed theory accounting for the formation of vortex polycrystals. The issue is particularly interesting since recent experiments indicate that the reentrant disordered vortex phase of NbS$_2$, commonly believed to be amorphous, is instead polycrystalline. Whether this is a stable thermodynamic phase is still an open question.

The theoretical description of vortex matter in high $T_c$ superconductors is centered on the role of quenched disorder. Early theoretical considerations seemed to imply that even a small amount of disorder would lead to the loss of long-range order and to the formation of an amorphous vortex glass phase. Experimental observations did not confirm this view, since ordered vortex structures are typically observed even in presence of disorder. This contradiction was resolved by a more detailed theoretical analysis of the weak disorder limit, showing a topologically ordered, long-range correlated phase, termed the Bragg glass. While the presence of a Bragg glass has been confirmed experimentally, the precise nature of the transitions into the amorphous and liquid phases is still debated. Recent theories highlight the importance of dislocations as mediators of the transition, in contrast with more traditional melting theories, based on the Lindeman criterion. The properties of dislocations in the vortex lattice have been the object of extensive theoretical investigations, but less is known about grain boundaries.

Here we address the problem of the formation of a vortex polycrystal from the point of view of grain growth. In field cooling experiments, magnetic flux is already present in the sample as it is quenched in the mixed phase. Thus it is reasonable to expect that vortices are originally disordered and that, due to their mutual interactions, undergo a local ordering process through the growth of grains with various orientations which, in turn, implies the annihilation of several dislocation lines as well as their organization into grain boundaries separating the crystalline grains (see Fig. for an example). The effect of quenched disorder is to pin the grain boundaries, hindering the growth process. Thus to understand the properties of vortex polycrystals, we analyze the dynamics of grain boundaries in vortex matter as they interact with disorder.

We first use continuum anisotropic elasticity to evaluate the elastic response of an extended three dimensional grain boundary to small perturbations. In the large-wavelength limit, the grain boundary elastic energy is found to be strongly non-local, with a linear wave vector dependence in Fourier space. Hence, it is not feasible to use a surface-energy approximation similar to the line-tension approximation frequently used to describe the
elastic response of isolated dislocations. We thus use the non-local elastic energy in the framework of weak and strong pinning theories and estimate the grain size of a vortex polycrystal. Our results are in good agreement with the experiments, reproducing the dependence of the grain size on the applied magnetic field found in NbMo single crystals. In addition, we discuss the effect of thermal activation and the associated creep laws.

The elastic energy of the vortex lattice can be expressed in terms of the vortex displacement field \( u \)

\[
\mathcal{H} = \frac{1}{2} \int d^3 r \left[ c_{11} (\nabla u)^2 + (c_{11} - c_{66}) (\nabla \cdot u)^2 + c_{44} (\partial_z u)^2 \right],
\]

where \( c_{11}, c_{44} \) and \( c_{66} \) are respectively the compression, tilt and shear moduli, and we assume the applied field to point along the \( z \) direction. In the simplest continuum and non-dispersive approximation the elastic moduli can be estimated as \( c_{11} \approx c_{44} \approx B^2/4\pi \) and \( c_{66} \approx \Phi_0 B / (8\pi \lambda)^2 \), where \( B \) is the magnetic induction, \( \Phi_0 \) is the magnetic flux quantum and \( \lambda \) is the London penetration length.

We describe an extended grain boundary as an infinite array of edge dislocations arranged regularly along the \( y \) axis, with spacing \( D \) and Burgers vector in the \( x \) direction. Note that due to the columnar grain structure of the vortex polycrystal, tilt and mixed boundaries which would require a more complicated description in terms of screw and edge dislocations, cannot occur. To obtain the elastic response of the grain boundary to small perturbations, we consider a generic deformation \( v = \mathbf{v}_n(z) \mathbf{x} \) for the \( n \)th dislocation along its glide plane and find the elastic displacements solving the elastic equation associated with Eq. 1 with the appropriate constraints induced by the dislocations. The grain boundary elastic energy can then be obtained as in Ref. 21 by a suitable expansion of Eq. 1. The full calculation is somewhat involved and will be reported in detail elsewhere. Here we just quote the resulting elastic energy which in Fourier space reads

\[
\mathcal{H}_{GB} = \frac{\pi b^2}{2D^2} \sum_{G_y} \int \frac{dQ_y}{2\pi} \int \frac{dk_z}{2\pi} M(Q_y + G_y, k_z) |\mathbf{v}|^2, \tag{2}
\]

where the sum is over the reciprocal vectors \( G_y \equiv 2\pi n/D, |\mathbf{v}|^2 = \mathbf{v}(Q_y, k_z) \mathbf{v}(-Q_y, -k_z) \) and the interaction kernel is given by

\[
M(k_y, k_z) = 2 c_{66} |k_y| + \frac{c_{44}}{c_{66}} k_z^2 \left[ \frac{2 k_y^2 + c_{44} k_z^2}{\sqrt{k_y^2 + c_{44} k_z^2}} \right]^2 - 4k_y^2 \sqrt{k_y^2 + c_{44} k_z^2} - 2 \left( \frac{c_{44}}{c_{66}} - \frac{c_{44}}{c_{11}} \right) |k_y| k_z^2. \tag{3}
\]

The long-distance behavior of the kernel is captured by the behavior at small wave vectors that is given by

\[
M(k_y, k_z) \simeq 2 c_{66} |k_y| + \sqrt{c_{44} c_{66}} |k_z|, \tag{4}
\]

corresponding to a long-range non-local interaction in real space. It is convenient to work in an isotropic reference frame, rescaling the \( y \) coordinate by a factor \( \xi = \sqrt{c_{44}/c_{66}} \). The elastic kernel then becomes \( M(k) \simeq K |k| \), with \( K \equiv \sqrt{c_{44} c_{66}} \). In thin films, we can neglect the deformations along \( z \) and the kernel is simply given by \( M(k) \simeq 2 c_{66} |k| \). Note that for an isolated vortex lattice dislocation it is correct up to a logarithmic factor to approximate the elastic energy by an effective line tension \( 2 c_{66} \), but a similar procedure is not possible for a grain boundary.

Quenched disorder induces elastic deformations of the grain boundaries and the competition between elasticity, disorder and a driving force acting on the boundary can be analyzed in the framework of pinning theories [1, 18]. Driving forces for grain boundary motion can be externally induced by a current flowing in the superconductor [25] or, as in our case, internally generated by the ordering process during grain growth [26]. Grain growth is driven by a reduction in energy: For an average grain size \( R \) and straight grain boundaries, the characteristic energy stored per unit volume in the form of grain boundary dislocations is of the order of \( \Gamma_0/R \), where \( \Gamma_0 \) is the energy per unit area of a grain boundary. Hence, the energy gain achieved by increasing the grain size by \( dR \) is \( \Gamma_0 R^2 dR \).

Physically, the removal of grain boundary dislocations occurs through the motion of junction points in the grain boundary network. As junction points must drag the connecting boundary with them, which may be pinned by disorder, motion can only occur if the energy gain at least matches the dissipative work which has to be done against the pinning forces. The dissipative work per unit volume expended in moving all grain boundaries by \( dR \) is \( \sigma_e (dR)/dR \), where \( \sigma_e \) is the pinning force per unit area. Balancing against the energy gain yields the limit
where \( R_a \) is the length at which the vortex displacements become of the order of the lattice spacing \( a \) and corresponds to the onset of the BG regime. The roughness exponent in the RM is estimated as \( \zeta_{RM} \approx 1/5 \). The pinning energy for the grain boundary is then given by \( \mathcal{H}_{pin} = \sum_n \int dx n_D(z) b \sigma_{xy}[v, nD, z] \). The roughness of the grain boundary can be obtained by a scaling argument \( 25 \) comparing this expression with the elastic energy in Eq. (2), yielding \( \zeta_{GB} = \zeta_{RM} \) in the RM regime and a logarithmic roughness for \( R > R_a \). Notice that both isolated dislocations and “dislocation bundles” are found to be rougher than grain boundaries \( 25 \), which implies that the latter are more stable.

The depinning stress can be computed within the framework of collective pinning theory: the energy associated with bending a grain boundary fraction of linear dimension \( L < R_a \) over the characteristic distance \( v \) can be estimated as

\[
\mathcal{E} = \frac{Kb^2}{D^2}Lv^2 - \frac{K\rho b}{D}Lv \left( \frac{L}{R_a} \right)^{1/5} + \sigma_b L^2 \varepsilon / D, 
\]

where the first term represents the elastic energy, the second the pinning energy, and the third the work done by an external driving stress \( \sigma \) in displacing the boundary. Minimizing the first two terms, for \( v = a \approx b \) \( 25 \), we obtain the “plastic” Larkin length \( L_p \approx (b/D)^2 R_a \), which is typically smaller than \( R_a \). The depinning stress is identified as the stress necessary to depin a section of dimension \( L_p \): \( \sigma_c = K b^2 / (D L_p) \). Combining this expression with Eq. (5), using \( \Gamma_0 \approx K b^2 / D \), we obtain \( R_g \approx R_a \). The identification of \( R_g \) with \( R_a \) was proposed in Ref. [12], but was not confirmed by experiments (see Fig. 2 and Ref. [27]). We therefore propose to interpret the experimental data under a strong pinning assumption.

Strong pinning: In this regime, pinning centers are strong and localized and one can assume that the dislocations forming the grain boundary are pinned by individual obstacles. We consider here the case of columnar defects, oriented along the z axis. This case should be relevant for the experiments of Ref. [12] where grain boundary pinning is provided by screw dislocations in the superconducting crystal. In these conditions, the problem becomes effectively two dimensional (2D) and we can directly generalize the strong pinning theory of Friedel \( 28 \), developed in the context of single dislocations, by taking into account non-local elastic interactions. The basic idea is to consider a grain boundary segment as it depins from a pair of strong obstacles. The length \( L \) of the segment corresponds to the effective spacing between obstacles along the grain boundary, and it forms a bulge of maximum width \( v \). After the grain boundary segment overcomes the pin it will travel by an amount which is, again, of the order of \( v \) and, hence, sweep an area of the order of \( L v \). At the depinning threshold, the grain boundary starts to move through a sequence of statistically equivalent configurations, and the freed segment will encounter, on average, precisely one new obstacle in the course of this process. This argument leads to the condition \( L v \approx \Gamma_0 / \rho \) where \( \rho \) is the area density of pinning defects. The elastic energy per unit length of the bulge of width \( v \) and extension \( L \) is \( 2c_{gb} b^2 v^2 / D^2 \) (2D result), and should balance the work per unit length \( \sigma_b L^2 \varepsilon / D \) done by the driving stress \( \sigma \) in bowing the boundary. This energy balance provides a relation between \( L \) and \( v \). Furthermore, at depinning the total force \( \sigma b L^2 / D \) should be equal to the defect strength \( f_0 \), where \( d \) is the sample thickness. Combining the equations above we obtain the depinning stress \( \sigma_c b = D f_0 / (d L_f) \), where the Friedel length \( L_f \) is given by \( L_f = 2c_{gb} b^2 d / (f_0 \rho D^2) \). Inserting the expression for the critical stress in Eq. (5) together with the scale-independent surface tension \( \Gamma_0 = 2c_{gb} b^2 / D \), we obtain

\[
\frac{R_g b}{c_{gb} b} \approx \frac{\xi^2 x b^3 d^2}{D^3 f_0 \rho}.
\]

In order to use this result to fit the data in Ref. [12], we have to express it in terms of the reduced field \( B \equiv B / H_{c2} \), where \( H_{c2} \) is the upper critical field of the superconductor. The field dependence is implicit in the parameters \( b \) and \( D \), i.e., \( b \sim D \sim a \sim B^{-1/2} \), as well as in the shear modulus \( c_{gb} \sim B \), and in the pinning strength \( f_0 \). The pinning force due to a screw dislocation was computed in Ref. [29], and is given by \( f_0 \propto B^{1/2}(1 - B) \ln(\xi / 2.7b_0B) \approx B^{1/2} \ln(\xi / 2.7b_0B) \), where \( \xi \approx 100 A \) is the coherence length \( 30 \), and \( b_0 \approx 5 A \) is the Burgers vector of the screw dislocation \( 29 \). The resulting expression predicts a linear field dependence of the grain size with logarithmic corrections. In Fig. 2 we can corroborate that the agreement of this prediction with magnetic decoration data from Ref. [12] is quite satisfactory, especially if compared to the estimate based on local elasticity assumptions.

In the discussion above we have neglected thermal fluctuations, which could induce an activated motion of the grain boundaries, particularly in high \( T_c \) materials. This problem can be approached generalizing scaling theories of creep for vortices and dislocations \( 1 \) \( 22 \). In the weak pinning regime, the relevant energy barrier that the grain boundaries have to surmount under an applied
stress $\sigma < \sigma_c$ is given by $U(\sigma) = U_0(\sigma_c/\sigma)^\mu$, where $U_0 \approx Kb^3R_a$ and $\mu = 1$. In our case, the applied stress is the ordering stress, so that we have $\sigma_c/\sigma \approx R/R_a$.

Using this expression in the energy barrier for thermally activated grain growth, it follows

$$\frac{dR}{dt} = R_a \exp \left[-\frac{U_0}{kT} \frac{R}{R_a}\right], \quad (9)$$

where $\tau$ is the appropriate characteristic time. The equation can readily be solved yielding, in the long time limit, a logarithmic growth $R(t)/R_a = kT/U_0 \log(t/\tau)$. This law holds for $R > R_a$ when the grain boundaries would be pinned at $T = 0$. In the initial growth stage $R \ll R_a$, we can neglect pinning forces and the dynamics is ruled by the ordering stress: $\dot{R} \sim 1/R$, yielding a power law growth $R(t) \sim \sqrt{t}$.

In conclusion, we have analyzed the problem of grain growth in a vortex polycrystal studying the dynamics of grain boundaries. We have obtained estimates for the grain size that compare well with experiments on NbMo crystals, and derived the law for thermally activated grain growth. In general, our theory should apply to field cooling experiments in which there is a competition between the ordering stress and the pinning stress. The resulting polycrystalline structure, at least in the weak pinning regime, represents a metastable state in which the system is trapped during its evolution towards the stable Bragg glass phase. The possibility of a thermodynamically stable polycrystalline vortex state, recently suggested by experiments [17] [31], still remains to be confirmed theoretically.

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