Field-driven topological glass transition
in a model flux line lattice

Seungoh Ryu
Dept. of Physics, Ohio State University, Columbus, OH 43021

A. Kapitulnik
S. Doniach
Dept. of Applied Physics, Stanford University, Stanford, CA 94305
(March 23, 2022)

Abstract

We show that the flux line lattice in a model layered high temperature superconductor becomes unstable above a critical magnetic field with respect to a plastic deformation via penetration of pairs of point-like disclination defects. The instability is characterized by the competition between the elastic and the pinning energies and is essentially assisted by softening of the lattice induced by a dimensional crossover of the fluctuations as field increases. We confirm through a computer simulation that this indeed may lead to a phase transition from crystalline order at low fields to a topologically disordered phase at higher fields. We propose that this mechanism provides a model of the low temperature field–driven disordering transition observed in neutron diffraction experiments on Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystals.
The mixed state in the high temperature superconductors (HTSC) has been studied from a wide variety of perspectives over the past few years [1]. Among the interesting issues under debates are the question of how vortices freeze [2,3] in the so-called vortex glass phase [4] as well as the nature of the melted phase [5,6]. In particular, one expects an intricate interplay of the underlying layered nature of the host material and the random point pins in shaping the nature of the frozen phase.

A recent decoration performed on both sides of the Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystal suggests that vortex lines maintain their line integrity at least at very low field [7]. On the other hand, the rapid disappearance of Bragg peak intensity in the recent small angle neutron diffraction (SANS) [8] has been interpreted by the authors in terms of decomposition of lines into pancake vortices [9]. A Lindemann-like criterion is usually invoked in discussing such a “decoupling theory” [10], but it fails to explain how the transition is brought about, if there is one.

Traditionally, the role of a pinning potential has been treated as a perturbation within the harmonic elastic framework. In the weak pinning limit, the perturbed lattice tries to optimize its free energy by forming elastic domains of correlated region with minimum elastic energy while it is fragmented in larger length scales to take advantage of the random potential energy [11,12]. Several attempts have been made recently to extend the simple dimensional argument [13,14] for length scales larger than the elastic volume, but without considerations of topological defects. Their effect is expected to dominate for strong enough disorder, resulting in a dislocation dominated “glass phase” [16,18].

In an earlier paper [19], we showed that the dramatic features of the SANS results can not be accounted for by a dimensional crossover alone of a “clean” lattice. We further suggested that the flux lattice in the highly anisotropic Bi$_2$Sr$_2$CaCu$_2$O$_8$ may suffer an instability against penetration of topological defects and therefore may deteriorate rapidly across a characteristic flux line density. More recently, such a transition has been claimed to be observed also in a YBa$_2$Cu$_3$O$_{7-δ}$ based superlattice [20]. In this letter, we report computer simulation studies of this transition using simulated annealing on a model flux line system.
We start by noting that when the density of flux line in a layered HTSC is varied, the effective anisotropy of the lattice and the disorder strength change. As a result, the elastic domains, described by an in-plane correlation length $R_d$ and an out of plane correlation length $L_d$ may shrink. In particular, when $L_d$ reaches the interlayer spacing, a new low temperature glass state that is dominated by disclinations appears. We propose that the transition to this phase is first order and is characterized by an explosive invasion of point-like disclination pairs across a horizontal line in the B-T phase diagram.

Employing a vortex representation of the Lawrence-Doniach model [21], we consider a stack of coupled two dimensional vortex lattices with pancake vortex coordinates $\{r_{i,z}\}$ with $i$ labelling the individual flux lines. An approximate pair-wise interaction under periodic boundary conditions has been derived to make large scale numerical calculations possible [22]. With a choice of in-plane penetration depth $\lambda(0) = 1800\,\text{Å}, d = 15\,\text{Å}, \kappa = 100$ and anisotropy $\gamma = \sqrt{M_c/M_{qb}} = 55$, we obtain, for a clean system, a melting line $T_m(B)$ which is in reasonable agreement with the experimental result [23]. The random potential is modelled by potential wells of uniform depth $U_p$, of radius given by the lesser of $2\xi_{ab}$ and the grid size scattered at random positions of each layer with an areal density of $n_p = 1/a_p^2 \equiv B_p/\phi_0$. We choose $U_p = 5\frac{d\phi_0^2}{8\pi^2\lambda^2(T)}$, $B_p = 150G$ in 16(SET #1) and 32(SET #3) layers which give the freezing temperature $\sim 40^\circ K$ for $1kG < B < 20kG$ under a Lindemann-like criterion in reasonable agreement with the experimentally determined irreversibility line $T_{irr}(B)$. We also have results for a different pin density $B_p = 2.4kG$ in 16 layers.(SET #2) The potential used in our simulation may be viewed as a coarse grained potential fluctuations with an unspecified microscopic origin. The line density($100G \sim 2kG$) was varied by changing sizes of grid cells and pin densities for a fixed number of vortices(64 lines in $L = 16$ or 32 layers) [22]. To obtain low temperature properties, we use a simulated annealing procedure starting with a perfect triangular lattice at $T = 1.3 \cdot T_f(B) \sim 50^\circ K$ and gradually decreasing $T$ with steps of $dT = 5^\circ K$ over 40,000 Monte Carlo steps. At $T = 4^\circ K$, additional 20,000 steps were performed to make measurement of physical quantities. This formally resembles a field-cooling procedure employed in typical measurements. The number of different pin
configurations was limited to five for each line density for practical reasons. The disclination charge density \( n_d(i, z) \) is measured every 50 steps through Delaunay triangulation performed in each layer to determine the coordination number \( Z \) of each vortex \[24\]. Then a charge of \( q = (Z - 6) \) is assigned to \( n_d(i, z) \).

**Results** In the inset to Fig. 1, we show the partial Fourier transform \( S(q_x, q_y, z = L) \) of the vortex density correlation function \( \int d^2\rho \exp[iq \cdot \rho] < n_v(\rho, z = L) \cdot n_v(0, 0) > \) as evaluated in our simulation where \( n_v(\rho, z) \) is the local vortex density. Ideally, SANS with \( q_x \sim 0 \) aims to measure \( \int dz S(q_x, q_y, z) \) and therefore for a macroscopic sample (\( L \rightarrow \infty \)), we expect it to be related to the diffraction pattern of \[8\]. The simulated Bragg peak intensities (dots in Fig. 1), decaying rapidly over a narrow range of \( \delta B/B_{cz} \sim 0.3 \), looks strikingly similar to the appropriately scaled data from Cubitt et al. The values of \( B_{cz} \) were 1800(Set #1) and 550(#2) Gauss while we used 500 Gauss for the experimental data. The statistical deviation of the intensity, \( \delta I_{G1}/I_{G1} \), over five disorder configurations is within 20 %. The nature of the apparent peak for Set #1 in the figure, therefore, can not be resolved at this time. To verify what is driving the rapid drop, we look into the behavior of topological defects and the fraction of pinned vortices, \( f_p \) which is given by \( \langle \sum_{i,z} \Theta(r_{i,z}) \rangle / N \) where \( \Theta(r) \) gives 1 if \( r \) is within any of the pinning wells and 0 otherwise. In Fig. 2, we observe a jump in \( f_p \) within the narrow range of \( \delta B/B_{cz} \sim 0.2 \), the same region over which the Bragg intensity vanishes. There is a corresponding increase in the total number of disclinations, \( \sum_{i,z} \langle |n_d(i, z)| \rangle \) accompanied by a rapid drop of the in-plane hexatic order parameter, \( \Psi_6 \) \[25\]. As shown in the inset to the low field side, a typical configuration has a finite number of defects, but they in general appear as neutral disclination pairs or quartets (equivalent to a bound pair of dislocations), healing each other over a finite length along \( z \)-axis. With these bound defects, the lattice order is disrupted only over a finite distance given by the size of these bound defects, and manifest itself as a distinct Bragg spots of Fig. 1. It is to be contrasted with the higher field configuration in which defects are threading from-top-to-bottom layers of the sample in various sizes and separations. In this phase, we find that the weak hexatic order is still present in each layer and that their correlation along the \( c \)-axis is
sensitively dependent on the overall strength of the pins \[26\].

Introducing an integer variable \( n_d^*(i, z) \) which gives 1 for a disclination and 0 otherwise for lattice site \((i, z)\), we define the probability distribution for length \( l \) of continuous defect lines:

\[
P(l) = \left[ \langle \sum_{i,z} \sum_q [1 - n_d^*(i, z_0)][1 - n_d^*(i, z_0 + l + 1)] \prod_{z = z_0 + 1}^{z_0 + l} n_d^*(i, z) \rangle \right],
\]

where \(< . . . >\) and \([ . . . ]\) mean thermal and defect averages, respectively. In a pin-free system, the distribution above \( T_m(B) \) shows a gradual crossover behavior as \( B \) increases, reflecting the underlying dimensional crossover of the fluctuations of the lattice \[23\]\[27\]. In this case of \( T \ll T_f \) with quenched disorder, however, we observe a more dramatic change which suggests a field-driven phase transition. In Fig. 3, we show \( P(l) \) of continuous defect length \( l \) for fields \( B/B_{cz} = 0.2 \sim 2 \) averaged over five different pin configurations(\#1). Despite large statistical fluctuations at the large tail, we can clearly see that \( P(l) \) for high field \( \sim e^{-\alpha l} \) qualitatively differs from the low field distribution for which \( P(l) = 0 \) for \( l > l_{\text{max}}(B) \). The exponential dependence for high field can easily be understood in terms of defects generated independently in each layer with a probability \( p \). A probability for an accidentally aligned line of length \( l \) will then be \( P(l) \sim (1 - p)^2p^{l/d} \sim \exp[-l/d|\log p]|. \) In the low field, the length of defect line is truncated by the energetic balance between the defect rigidity and the overall gain from random pins.

This observation gives a clue in understanding the role of pins in the defect representation of the free energy. Clearly, the pinning potential acts as an effective “temperature” to drive the topological defects into the lattice by encouraging vortices to make large excursions to seek optimal pinning configurations. The occurrence of these topological defects signals the breakdown of the elastic theory and the transition to a new defect-dominated phase. We can estimate the breakdown field \( B_{cz} \) as follows: Let us assume that the accumulated vortex displacements \( u_i(x) \) reach \( O(a_B) \) over a volume \( V_d \) of radius \( R_d \) in the \( ab\)-plane, length \( L_d \) along the \( c\)-axis. For \( B < [U_p/ed]^4B_p^2/B_J \), where \( B_J \equiv \phi_0/(\gamma d)^2 \), a variational minimization of elastic free energy yields \( R_d/a_B < 1 \), suggesting a breakdown of the quasi-crystalline order.
occurring in the low field region of the phase diagram. Consequently, we assume a very short ranged in-plane order and fix \( R_d \sim a_B \), and perform a partial variational calculation for a tube of variable length \( L_d |_{R_d \sim a_B} \) to obtain, \( L_d(B)/d \sim [\epsilon^2 d^2 B_j^2 / U_p^2 B_B B]^1/3 \). The breakdown field \( B_{cz} \) is obtained from the condition \( L_d(B_{cz}) < d \). Here we assume that the statistical gain in pinning energy by bending of such tubes is given by \( U_p(n_p V_d/d)^{0.5+\delta}/(a_B^2 L_d) \) with \( \delta = 0 \), a rough approximation. Using the parameter values we chose, this yields \( B_{cz} \sim 2.4 \text{kG} \),[Set #1] in reasonable agreement with the result of the simulation.

The results of the simulations may be summarized in a phase diagram given in Fig. 4. At low temperatures, the effective “noise temperature” of the random pinning field drives the system from a quasi-crystalline phase at low fields to a defect-dominated topologically disordered phase at higher fields. This phase transition is facilitated by weak interlayer coupling, thus explaining the small value of the critical field \( B_{cz} \) for highly anisotropic materials such as \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \). On the other hand, for less anisotropic materials such as \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \), this instability should be pushed to a higher field. Because the disorder is induced by the pins, the vortices are still highly localized, hence in a glassy phase. We have not yet used our simulations to study the kinetics of this phase, however, from our previous studies [28], we expect the kinetics of the phase to be sub-ohmic, so that it should still be a superconductor.

As the temperature is increased in the topologically disordered phase, we expect to reach a “depinning temperature” above which the defects become liquid-like and the transport would be ohmic. The exact shape of the line of phase transitions between the quasi-crystalline phase and the topological glass phase depend on the details of the competing energies and may terminate at the melting line \( T_m^{3d}(B) \) which was recently shown to bend toward and terminate at a field of \( \sim 500 \text{ Gauss} \) [29]. In the vicinity of the transition line \( B_{cz} \), the explosion of topological defects will be expected to dominate the kinetics and may provide an explanation of the “fishtail” peak-effect in the critical current observed as the B-field is varied in this region of the phase diagram [30][31]. The results reported here are reminiscent of a transition observed independently by Gingras and Huse from simulations.
of a ferromagnetic 3d XY model with a random field [32].

The authors are grateful for the support by EPRI and Air Force. SR was also supported by NSF Grant DMR94-02131, Midwest Superconductivity Consortium through DOE Grant DE-FG02-90ER-45427 and by Ohio State University Postdoctoral Fellowship. SR acknowledges very useful discussions with Dr. Forgan and Dr. Stroud.
REFERENCES

[1] G. Blatter, M. V. Feigel’man, V. B. Geshkenbein, A. I. Larkin, and V. M. Vinokur. *Rev. Mod. Phys.*, **66**, 1125, (1995).

[2] C. A. Murray, P. L. Gammel, D. J. Bishop, D. M. Mitzi, and A. Kapitulnik. *Phys. Rev. Lett.*, **64**, 2312, (1990).

[3] E. M. Chudnovsky. *Phys. Rev. B*, **40**, 11355, (1989).

[4] M. P. A. Fisher. *Phys. Rev. Lett.*, **62**, 1415, (1988).

[5] D. R. Nelson. *Phys. Rev. Lett.*, **60**, 1973, (1988).

[6] M. C. Marchetti and D. R. Nelson. *Phys. Rev. B*, **42**, 9938, (1990).

[7] Z. Yao, S. Yoon, H. Dai, S. Fan, C. M. Lieber. *Nature*, **371**, 777, (1995).

[8] R. Cubitt, E. M. Forgan, G. Yang, S. L. Lee, D. M. Paul, H. A. Mook, M. Yethiraj, P. H. Kes, T. W. Li, A. A. Menovsky, Z. Tarnawski, and K. Mortensen. *Nature*, **365**, 407, (1993).

[9] J. R. Clem. *Phys. Rev. B*, **43**, 7837, (1991).

[10] A. Schilling, R. Jin, J. D. Guo, and H. R. Ott. *Phys. Rev. Lett.*, **71**, 1899, (1993).

[11] Y. Imry and S.-K. Ma. *Phys. Rev. Lett.*, **35**, 1399, (1975).

[12] A. I. Larkin and Y. N. Ovchinnikov. *J. Low Temp. Phys.*, **43**, 109, (1979).

[13] J.-P. Bouchaud, M. Mezard, and J. S. Yedidia. *Phys. Rev. B*, **46**, 14686, (1992).

[14] T. Nattermann. *Phys. Rev. Lett.*, **64**, 2454, (1990).

[15] T. Giamarchi and P. L. Doussal. *Phys. Rev. Lett.*, **72**, 1530, (1994).

[16] D. A. Huse, *Physica B*, **197**, 540, (1994).

[17] Seungoh Ryu, *Computer simulation studies of flux lines in a model layered supercon-
ducitor, PhD thesis, Stanford University, (1994). See chapter [10].

[18] T. Giamarchi, P. Le Doussal. Phys. Rev. B, 52, 1242, (1995).

[19] S. Ryu, S. Doniach, and A. Kapitulnik. SPIE Proceedings, 2157, 12, (1994).

[20] H. Obara, M. Anderson, L. Fàbrega, P. Fivat, J.-M. Triscone, M. Decroux, Ø. Fischer. Phys. Rev. Lett., 74, 3041, (1995).

[21] W. E. Lawrence and S. Doniach, 1971, in Proceedings of LT12, Kyoto, Japan, edited by E. Kanda, (Keigaku, Tokyo), p. 361.

[22] S. Ryu, S. Doniach, G. Deutscher, and A. Kapitulnik. Phys. Rev. Lett., 68, 710, (1992).

[23] See Chapters 5-6 and 8 of [17].

[24] D. R. Nelson. In C. Domb and J. L. Lebowitz, editors, Phase transitions and critical phenomena, vol.7. Academic Press, New York, (1983).

[25] After Delaunay triangulation, the local hexatic order parameter is evaluated from

\[
\Psi_6 = \frac{1}{N} \langle \sum_{ij'z} \frac{1}{c_{i,z}} \exp[i6\theta_{ij}(z)] \rangle
\]

where \(N\) is the total number of pancakes, \(c_{i,z}\) is the coordination number of a pancake, \(\theta_{ij}(z)\) is the bond angle between neighbouring pancakes measured with respect to a fixed direction, \(\hat{x}\).

[26] For \(B_p = 150G\), we have \(|\Psi_6|^2 \sim 0.2\) with \(<\Psi_6(z)\Psi_6(z-1)^*\sim 0.2\), while for \(B_p = 2.4kG\), they were 0.1 and 0.01 at the field where the Bragg peak intensity vanishes. Both \(\Psi_6\) and its interlayer correlation monotonically decreases as field further increases. We note that the kink observed in the pinned fraction around \(B \sim 5B_{cz}\) could possibly signal the occurrence of an intermediate phase.

[27] Seungoh Ryu and D. Stroud, to be published in Phys. Rev. B, (1996).

[28] Seungoh Ryu, A. Kapitulnik, and S. Doniach, Phys. Rev. Lett., 71, 4245, (1993).

[29] E. Zeldov, D. Majer, M. Konczykowski, V. B. Geshkenbein, V. M. Vinokur, H. Shtrik-
man, *Nature*, **375**, 373, (1995).

[30] Y. Yeshurun, N. Bontemps, L. Burlachkov, A. Kapitulnik, *Phys. Rev. B*, **49**, 1548, (1994).

[31] K. A. Moler, G. Roos, L. W. Lombardo, J. S. Harris, and A. Kapitulnik, *to be published*.

[32] M. J. P. Gingras and D. A. Huse. preprint, (1995).

[33] M. C. Hellerqvist, S. Ryu, L. W. Lombardo, and A. Kapitulnik. *Physica C*, **230**, 170, (1994).
FIGURES

FIG. 1. The relative integrated intensity of the first order Bragg peak in the partial structure factor for Set #1 and #2. The intensity was normalized by that of the clean sample at the same temperature and field. The broken line is from the Neutron scattering data [8] drawn with an arbitrary scale. The field was arbitrarily scaled by a value at which the intensity reaches the flat bottom. The insets show the simulated diffraction pattern for three representative points (labelled a,b,c) of Set #1 in the curve. Intensity for (c) was multiplied by a factor of 30.

FIG. 2. Pinned fraction of vortices across the instability line for Set #1. The broken line is a guide showing the naive trend of $\sim B_p/B$ as expected from the relative ratio of the densities. The abrupt increase in the pinned fraction is closely accompanied by the proliferation of topological defects as shown as black ($z > 6$) and gray ($z < 6$) dots in the insets.

FIG. 3. $P(l)$ for various values of $B$ averaged over five different realizations of pins (Set #3). Number of layers was 32. Filled circles correspond to the hexatic glass region while open symbols are for higher field topological glass regime. Broken lines are guides for the eye.

FIG. 4. Schematic phase diagram with strong point pins. The low field elastic lattice is turned into a topological glass state as $B$ increases over $B_{cz}$. The freezing temperatures ($T_{f}^{3d}$ and $T_{f}^{2d}$) are characterized by the dimensionality of topological defects as discussed in the text. We also note that there is a distinct decoupling crossover line $T_{dc}$ in the liquid phase across which the vortex lines disintegrate into pancake vortices through cutting and reconnection [33].