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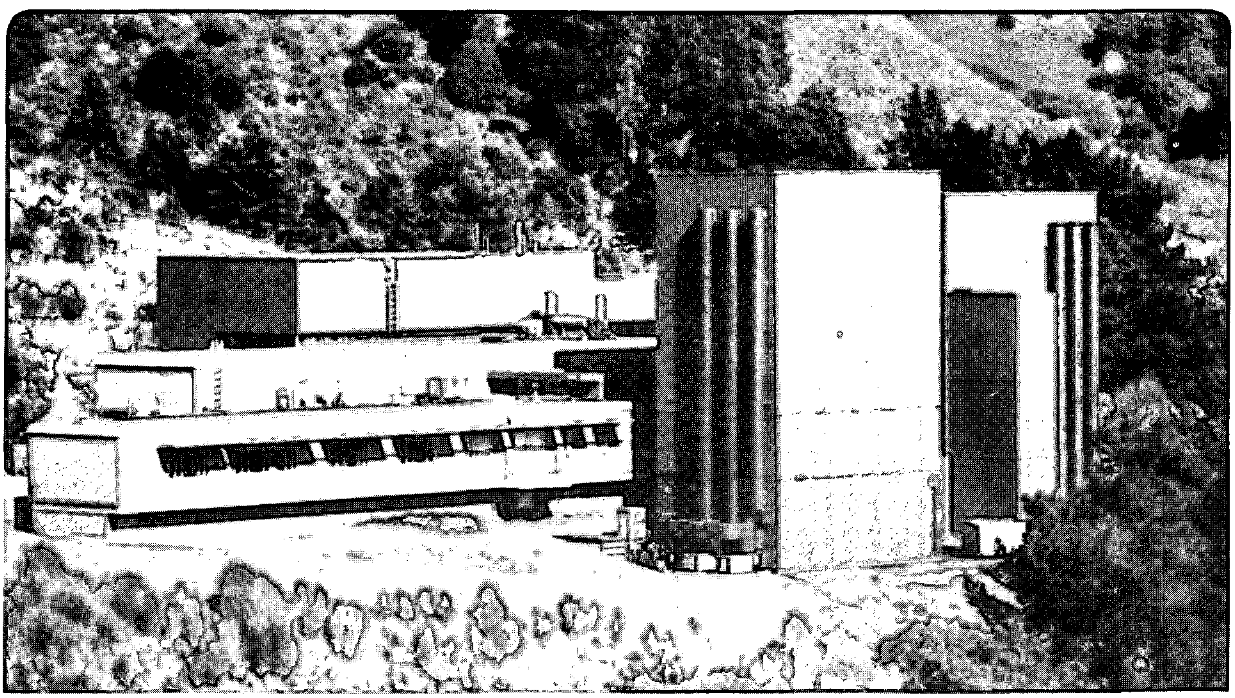

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Simulation of vortex-line pinning by defects in the Y-Ba-Cu-O system.

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ABSTRACT

The finite temperature properties of a two-dimensional flux lattice are studied by Monte Carlo simulation, with particular attention to the effects of twin-boundaries. The parameters selected are appropriate for the $YBa_2Cu_3O_7$ high-temperature superconducting system. The intrinsic properties of the vortex state are investigated by monitoring system evolution at fixed temperature and applied magnetic field. By varying the temperature, the loss of type-II superconductivity via fluxoid lattice melting is also examined. The introduction of model defects induces the creation of metastable and glassy states which reduce overall hexatic order but are found to enhance system resistance to flux-lattice melting.

INTRODUCTION

The $YBa_2Cu_3O_{7-\delta}$ high temperature superconductor has been the source of much activity in recent years. With a critical temperature (T_c) above the boiling point of liquid nitrogen (for $\delta < 0.3$), it promises to allow the use of superconductivity in many commercial applications some of which involve the use of high field (> 10^6 Gauss) magnets. However, the $YBa_2Cu_3O_{7-\delta}$ superconductor has a relatively poor intrinsic magnetic critical field (H_{C2}) due to the phonon-induced magnetic fluxoid lattice melting, which limits its applicability for many purposes. Standard approaches to producing "hard" superconductors with higher H_{C2} involve the introduction of suitable structural defects which couple with the individual magnetic fluxoids, effectively pinning the flux lattice and sustaining type-II superconductivity to higher critical magnetic fields. A number of such defects that enhance H_{C2} in the Y-Ba-Cu-O system have been reported in the literature. Examples include: twin-boundaries[1], dislocations[2], grain boundaries[3], Y_2BaCuO_5 inclusions[4], and stacking faults due to $YBa_2Cu_4O_8$ inclusions in an $YBa_2Cu_3O_7$ matrix[5,6]. The nature of the flux lattice in the copper-oxide superconductors continues to be the subject of active debate and was recently reviewed[7,8]. It is now generally accepted that the Abrikosov lattice normally expected is easily destroyed in the high-temperature superconductors because of strong thermal fluctuations leading to a vortex fluid proposed by Nelson and Seung[9]. In addition, it had been known since the pioneering work of Larkin and Ovchinnikov[10] that random pinning centers lead to a destruction of the long-range order, but it was argued by Fisher[11] that the resulting pattern may still possess considerable orientational order, leading to a glassy vortex phase, for which there is now increasing evidence. Recently, much computer simulation work at different levels of approximation has been performed to elucidate these questions[12-17]. The ultimate aim of the present study is to investigate the effects of realistic defect distributions obtained from a prior computer simulation[5,18] of the appropriate structural transformations. As a first step in this direction, in the present work flux pinning defects are distributed in various configurations and the nature of fluxoid lattice melting under different conditions is examined.

THEORY OF VORTEX LATTICES

The $YBa_2Cu_3O_{7-\delta}$ superconductor, has the ratio of magnetic penetration depth, λ, to coherence length, ξ, larger than $1/\sqrt{2}$, in fact $\kappa = \lambda/\xi \approx 100$, and therefore displays type-II behavior. Fluxoid penetration in type-II materials is described phenomenologically by the Ginzburg-Landau theory and quantitatively (at least in the regimes studied here) by the London equations. For type-II superconductors, the magnetic field penetrates the superconducting material in quantized flux units, $\Phi_0 = hc/2e = 2.07\times10^{-7} Gauss\text{-}cm^2$, in the direction of the applied magnetic field. The internal magnetic field density about a fluxoid as a function of radial distance, R, derived by solution of the London equations for constant applied field, takes the form

$$B(R) = \frac{\Phi_0}{2\pi\lambda^2} K_0(R/\lambda) \quad (1)$$

where λ is the magnetic field penetration depth and K_0 is the modified Bessel function of the first order. Within the material, the contribution to the internal energy due to the fluxoids is:

$$U = \frac{(\Phi_0)^2}{8\pi^2\lambda^2} \sum_{i \neq j}^{N} K_0(R_{ij}/\lambda) \tag{2}$$

where R_{ij} is the radial separation of a pair of fluxoids. The quantity

$$\frac{(\Phi_0)^2}{8\pi^2\lambda^2} = U_0 \tag{3}$$

is taken to be the unit of energy and is set to unity for simulation purposes.

MONTE CARLO TECHNIQUE

To investigate the behavior of the flux lattice at a given temperature, external field or defect arrangement, Monte Carlo simulations have been performed. In the canonical scheme used here, the internal applied magnetic field is specified by the flux density chosen for the simulation, Φ_0/A. As interactions with the form of the modified Bessel function are long ranged in the regime of type-II superconductivity, the simulation is performed with periodic boundary conditions with image lattices taken over the distance of appreciable interaction strength for the applied field.

The present work is restricted to a study of two-dimensional flux lattices, appropriate for thin films. In the Monte Carlo scheme according to the Metropolis algorithm[19] a flux line is randomly selected and an attempt is made to displace it over an amount $\Delta\mathbf{r}$. This displacement is generated as a pair of Cartesian coordinates $(\Delta x, \Delta y)$ where both Δx and Δy are randomly selected to lie in the interval [-100, 100], all distances henceforth being measured in Å. The change in internal energy ΔU associated with this displacement is calculated and the move is executed provided that $exp[-\Delta U/k_B T] > p$ where p is a random number in the interval [0,1], k_B is Boltzmann's constant, and T the absolute temperature. This procedure is repeated many times until the coarse grain energy has settled down to a constant value, corresponding to thermodynamic equilibrium. In this state averages are calculated to determine the specific heat:

$$c_v = N^{-1}(<E^2> - <E>^2)/kT^2 \tag{4}$$

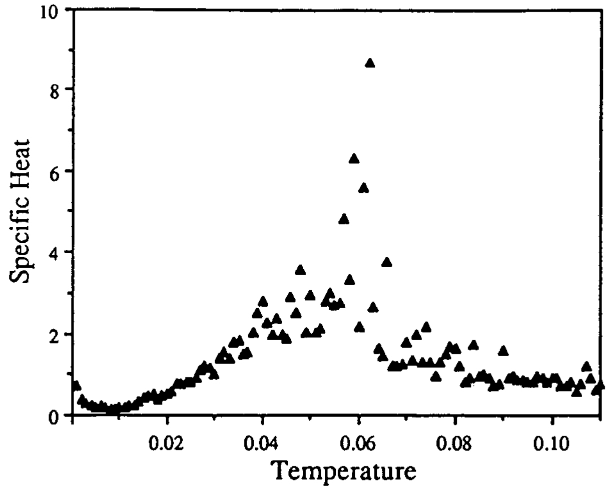
where N is the number of vortices and the angular brackets denote an ensemble average. Near a phase transition the specific heat goes through a maximum. Another useful quantity to characterize the state of order is the hexatic order parameter defined as:

$$\psi_6 = <\sum_{j=1}^{6} exp[i\,6\theta_j(r_j)]> \tag{5}$$

where θ_j is the angle between a fluxoid and its nearest neighbor j, the sum runs over the six nearest neighbors, and the average is taken over all vortices. The magnitude of this quantity is equal to 1 for a perfect hexagonal (Abrikosov) lattice and approaches zero for large deviations from hexagonal symmetry. In all calculations discussed here 30 flux lines were placed inside a simulation cell having dimensions 5000 Å by 5000 Å with periodic boundary conditions. This corresponds to an internal magnetic field of 2,484 Gauss. Starting from an arbitrary initial arrangement, typically 30,000 simulation iterations were allowed to elapse for system equilibration before statistical averages were taken.

RESULTS AND DISCUSSION

Monitoring the specific heat of the system and varying temperature, a peak corresponding to the fluxoid lattice melting temperature is detected at $T = 0.06 k_B/U_0$ for an internal magnetic field of 2,484 Gauss [Figure 1a]. Taking the two-dimensional fluxoid lattice to be a 3.5 Å slice of a three-dimensional simulation, this corresponds to a temperature of approximately $T = 81.5K$, in good agreement with values reported experimentally[20]. The hexatic order parameter is also observed to fall statistically to zero at this temperature, indicating a loss of hexagonal symmetry at the melting temperature, as expected [Figure 1b].



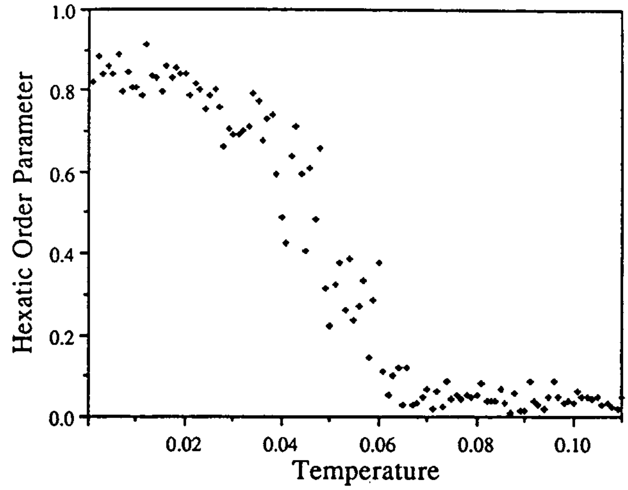


Figure 1: Thermodynamic indications of fluxoid lattice melting. **(a)** Specific heat versus temperature for a system of fluxoids simulated at constant magnetic field of 2,484 Gauss. Data presented is unaveraged to illustrate the scatter due to metastable *glassy* state contributions. The peak in the specific heat, corresponding to melting of the fluxoid lattice, appears at the simulation temperature of $T = 0.06k_B/U_0$. Low temperature non-zero tail is due to frozen-in glassy states. **(b)** Hexatic order parameter versus temperature corresponding to runs depicted in Figure 1a. Drop to zero corresponds to a loss of hexatic order at the melting temperature.

In order to further examine the undefected state, the dynamics of the simulated fluxoid lattice were studied at temperatures well below, at, and well above the melting temperature by tracing the motion of the individual fluxoids over 100 attempted displacements per site once coarse grain energy averages indicated that equilibrium had been achieved. At temperatures well below the melting point ($T = 0.025k_B/U_0$), a highly ordered hexagonal lattice is obtained [Figure 2a]. Fluxoid motion is quasi-harmonic and confined to a small region about the equilibrium position. The effect of the square boundary conditions can be seen in the alignment of the [1000] planes with the edge of the simulation unit cell, depicted by the border. At the melting temperature [Figure 2b], the lattice still retains significant order but the average displacement of the fluxoids is much greater than that at lower temperatures. Preliminary analysis indicates that the mean square deviation of the particles is consistent with the Lindemann criterion for melting, but a careful study of the finite size effects and possible hysteresis remains to be done to fully warrant this conclusion. At $T = 0.1k_B/U_0$, well above the melting point, no significant order is apparent and the fluxoids form a liquid with average displacement greater than the former equilibrium lattice spacing [Figure 2c].

It has been reported (see Ref. 8 and references therein) that the $YBa_2Cu_3O_{7-\delta}$ superconductors, due to their highly defected intrinsic state, are not expected to develop well ordered hexagonal fluxoid lattices in the mixed superconducting state. Instead, interactions of both attractive and repulsive nature of the fluxoid lattice with defects lead to a "glassy" fluxoid state which has remnant hexatic order. In order to assess the nature of defects sufficient to induce a glassy mixed state, model planar defects were introduced into the simulation unit cell. In a first approximation, the planar defect potential was taken to be a square trough potential with a binding energy of $-20U_0$ and a width of 100 Å . This can be viewed as a simple model for a twin-boundary, although other forms of interaction could be envisioned (see e.g. Ref. 13)

A single defect introduced into the simulation cell has little effect on the overall behavior of the system as the lattice is able to accommodate the defect by establishing its [1100] planes parallel to the planar defect. In some cases, an extra fluxoid is trapped by the boundary [Figure 3a]. This results in a vacancy in the surrounding lattice and a significant decrease in hexatic order. As the thermal contribution to the lattice energy increases, the pinning effect of the boundary is enhanced and a larger number of vortices are trapped [Figure 3b]. The resulting excess magnetic field in the region repels nearby fluxoids and creates an adjacent flux-free region.

Notice in Figure 3b the path of a fluxoid which is just trapped into the defect region. At temperatures above the melting point of the undefected system, significant remnant order is observed [Figure 3c]. The effect of the pinning boundary is to stabilize the lattice to slightly higher temperatures even while decreasing the overall order in the " solid" state. An increased number of fluxoids are trapped by the boundary leading to a linear region of high fluxoid concentration adjacent to a region of lower magnetic field, itself bounded by a region of fluxoid " liquid". The fluxoids trapped at the planar defect act as a grain boundary in the flux lattice and provide a channel of high mobility for the vortices thus lowering the temperature at which flux lines start to diffuse, in a mechanism similar to that found by Jensen et al.[12] in a study of randomly distributed pinning centers.

In the case of multiple defects, this trend is even more apparent. Two planar defects placed 3500 Å apart, a distance incommensurate with the primary [1000] and [1100] lattice spacings at the magnetic field under study, gives rise to a loss in hexatic order at temperatures below the melting temperature of the undefected system. However, once the lattice has distorted to accommodate the presence of defects, the resulting structure retains significant remnant hexatic order, raising the melting point of the defected system to slightly higher temperatures. At low temperatures, the system accommodates the two defects with minor distortion of the Abrikosov lattice as the mean displacement of each vortex does not exceed the width of the boundary [Figure 4a]. However, at higher temperatures [Figures 4b and 4c], the defects are clearly constraining the defect free regions to maintain a degree of hexatic order greater than that of the undefected system at the same temperature. This can be best seen by comparing Figure 4c to Figures 2c and 3c. It is felt that this remnant order, imposed by the attractive effect of the defects, reflects a stabilization of the vortex state in the presence of pinning defects. Indeed, initial simulation results suggest that the melting temperature of a lattice containing fluxoid pinning defects increases compared to the undefected lattice.

CONCLUSIONS

In summary, Monte Carlo simulations of a two-dimensional arrangement of fluxoids with parameters appropriate for Y-Ba-Cu-O have been performed, with particular emphasis on the effects of

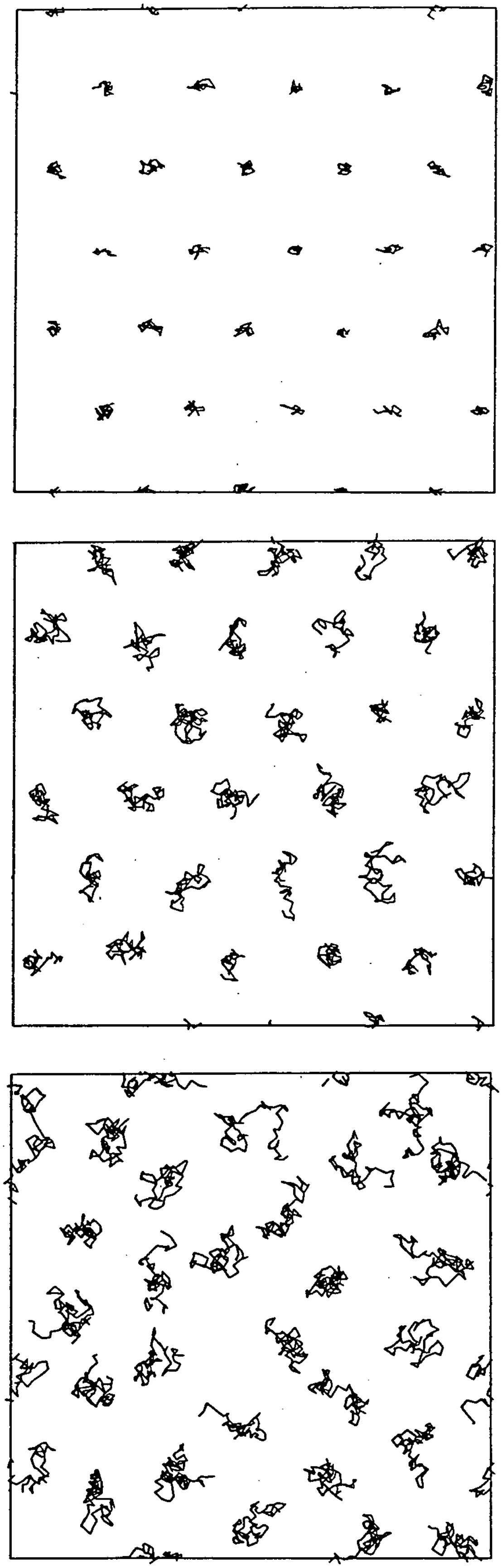


Figure 2: Trace of undefected vortex lattice motion at various temperatures. See text for discussion. **(a)** $T = 0.025 k_B T / U_0 < T_m$. **(b)** $T = 0.06 k_B T / U_0 \approx T_m$. **(c)** $T = 0.01 k_B T / U_0 > T_m$.

planar defects. Flux lattice melting and a "glassy" phase in the presence of defects have been observed. The results are consistent with a Kosterlitz-Thouless phase transition but further calculations are being performed to judge finite size effects and analyze the possibility of a smeared first-order transition. It needs to be pointed out that the paths of flux motion obtained in a Monte Carlo simulation, although enlightening, need to be interpreted with care as they do not necessarily reflect true dynamics. More realistic dynamic information could be obtained by using a combined molecular dynamics simulated annealing technique[12,14], but this would involve much more time consuming calculations. The model could easily be extended to deal with other superconducting materials. This may involve going beyond the London approximation and solving the time-dependent Ginzburg-Landau equation[21] or solving the London equations numerically for a spatially dependent penetration depth[14], $\lambda(r)$. Also for direct experimental comparison the extension to three-dimensional lattices including flux cutting[22] may be necessary. However, the present calculations demonstrate the feasibility of a combined simulational approach, in which realistic defect arrangements are obtained from a structural Monte Carlo simulation and are subsequently used as the medium in which flux lattice phenomena are studied. Results of such an approach will be reported in the near future.

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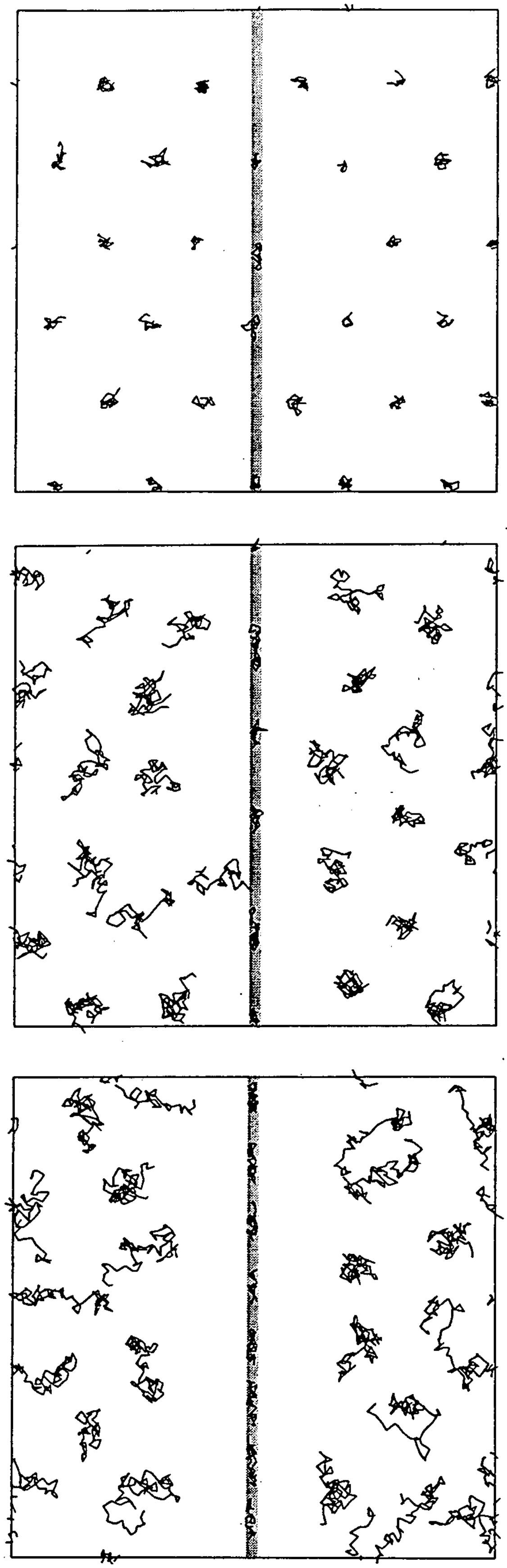

Figure 3: Trace of vortex lattice motion at various temperatures under the influence of one linear fluxoid pinning defect. See text for discussion. **(a)** $T = 0.025 k_B T / U_0 < T_m$. **(b)** $T = 0.06 k_B T / U_0 \approx T_m$. **(c)** $T = 0.01 k_B T / U_0 > T_m$.

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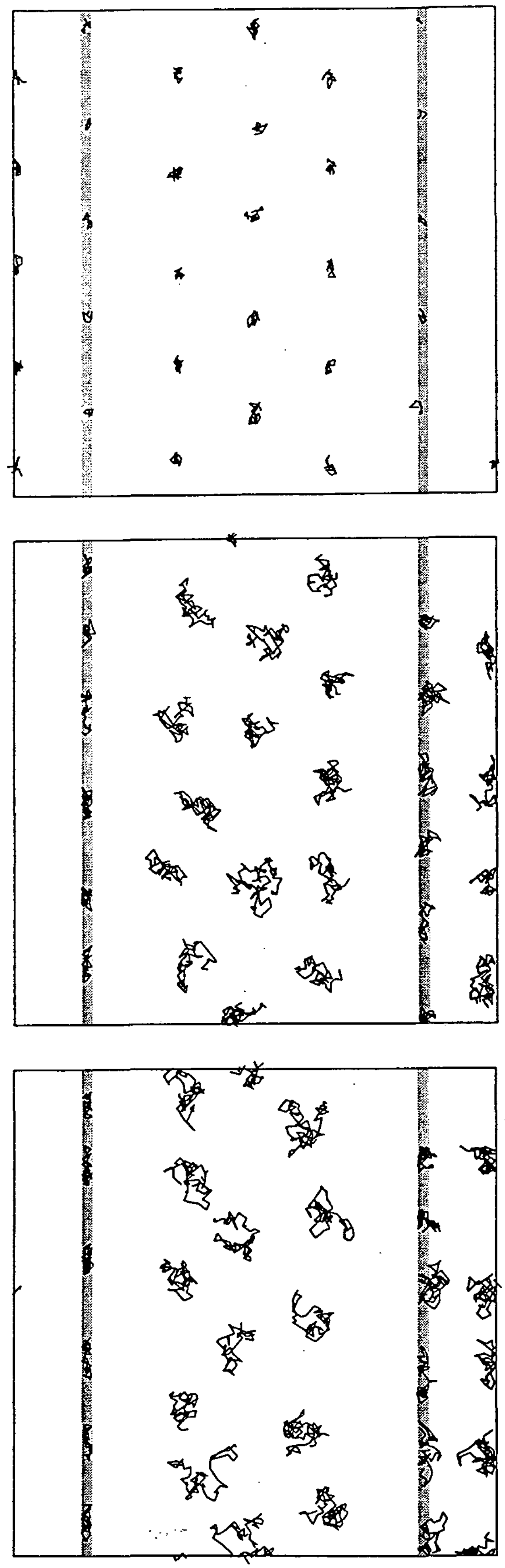

Figure 4: Trace of vortex lattice motion at various temperatures under the influence of two linear fluxoid pinning defects. See text for discussion. **(a)** $T = 0.025 k_B T / U_0 < T_m$. **(b)** $T = 0.06 k_B T / U_0 \approx T_m$. **(c)** $T = 0.01 k_B T / U_0 > T_m$.