Lattice Deformations and Plastic Flow through Bottlenecks in a Two-Dimensional Model for Flux Pinning in Type-II Superconductors

H. J. Jensen, A. Brass, and A. J. Berlinsky
Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada L8S 4M1
(Received 12 August 1987)

The deformations of a 2D vortex lattice pinned by a random potential are studied by a molecular-dynamics annealing method. All but very weak potentials produce a highly defective lattice, consisting of trapped lattice regions separated by channels in which the vortices flow plastically. It is argued that this type of deformation is the cause of the observed restricted applicability of collective pinning theory.

PACS numbers: 74.60.Ge, 61.40.+b, 62.20.Fe

The statistical summation of random attractive forces acting on a deformable lattice is a general problem relevant to flux pinning in type-II superconductors as well as to other phenomena such as the pinning of charge-density waves. The nature of deformations induced by the random potential is of crucial importance and can fall into three general classes, depending on the strength of the potential. For very weak pinning, only elastic and reversible deformations of the lattice occur. However, the size of this weak-pinning region shrinks to zero for a macroscopic system. An intermediate regime exists, in which elastic instabilities are induced but not plastic deformations. The collective pinning theory of Larkin and Ovchinnikov[1] applies only to this region. Finally, there exists a plastic region, in which we find that pinning centers trap individual lattice particles, and the lattice becomes highly defective as plastic flow starts to take place in between pinned regions. This region has been shown to be experimentally relevant for superconducting films.[2]

The theory of Larkin and Ovchinnikov was investigated numerically by Brandt,[3] who found it to be applicable in the region of elastic instabilities and, surprisingly, sometimes even for stronger pins. However, Brandt did not investigate the actual deformations of the lattice in detail. We have studied the lattice deformations numerically using a molecular-dynamics (MD) annealing method to relax the lattice in the presence of a random pinning potential. We find that the elastic instability region is very narrow and that the results obtained for larger pinning strengths depend critically on the degree of relaxation. Especially for pinning strengths near the crossover between the elastic instability region and the plastic region, we find that Brandt's simulation method suffers to some extent from insufficient relaxation.

Our system consists of N_v vortices with variable positions $\mathbf{r}_i=(x_i,y_i)$ and N_p pins with random position $\mathbf{r}_i^{(p)}$ in an area $A=L_xL_y$ with periodic boundary conditions. The potential energy of the system is given by

$$U=\sum_{i\neq j}V_v(|\mathbf{r}_i-\mathbf{r}_j|)+\sum_{i,j}V_p(|\mathbf{r}_i-\mathbf{r}_j^{(p)}|), \qquad (1)$$

$$V_v(r)=A_v v(r/R_v), \quad V_p(r)=A_p v(r/R_p),$$

where $v(\rho)$ is a Gaussian-type potential. The units are fixed by the choice $A_v=1$ and the ideal vortex lattice spacing $a_0=1$. Our simulations are made on systems consisting of 56, 340, or 1200 vortices with $R_v=0.6$ or 0.75 corresponding to a shear modulus $C_{66}=0.2695$ or 0.08306 and a compression modulus $C_{11}=1.9943$ or 2.5215. The number of pins is $N_p=73$, 146, and 438 with $-1.0\leq A_p\leq -0.01$ and range $R_p=0.125$, 0.25, and 0.5.

The main difference between the simulations presented here and those of Ref. 3 is in the method used to relax the lattice. The simulations in Ref. 3 were produced by direct relaxations of the potential energy of the lattice. We find that such direct relaxations have a pronounced tendency to become stuck in metastable local minima. The relaxation technique employed in the present work is a MD annealing method. In order to apply the MD technique, we add an auxiliary kinetic term to the potential (1), and we study $H=T+U$ at very low temperature. A unit mass is ascribed *ad hoc* to each vortex. In this method, energy is extracted or added in the form of kinetic energy, and the system then repartitions kinetic and potential energy by following its equation of motion.

The initial relaxation is performed by a gradual cooling down of the vortices from a temperature of about $0.1|A_p|$ to $(10^{-4}\text{–}10^{-5})|A_p|$. The cooling is achieved by our gradually scaling the vortex velocities down. As the temperature drops, we let the cooling rate decrease to improve the relaxation. When the relaxed state has been reached, we shift the center of mass (c.m.) of the vortices over the pins in the ⟨10⟩ direction by shifting all the vortices by a small increment $dx=10^{-4}$ to 10^{-3} (the smaller increment is used for the strongest pins). We then let the vortices relax by the MD procedure for ten time steps, keeping the temperature fixed at the low temperature reached in the initial cooling. The c.m. is kept fixed during this relaxation by the subtraction of the c.m. velocity at the end of each time step. This procedure amounts to the application of an external homogeneous driving force so as precisely to balance out the pinning force at any instant. We continue the procedure of successively shifting and relaxing the lattice until the c.m. has been shifted a distance between 0.25 and 1.2

lattice spacings. The more complete relaxation achieved in this way has allowed us to observe the pulsating flow and sawtoothed force laws described below which are easily missed if relaxation is incomplete.

The changes in the potential energy, caused by a shift, are given by

$$\Delta U = \sum_i \frac{\partial U}{\partial \mathbf{r}_i} \cdot d\mathbf{x}_i = -\sum_i \frac{\partial V_p}{\partial \mathbf{r}_i^{(p)}} \cdot d\mathbf{x} = -\mathbf{F} \cdot d\mathbf{x} \qquad (2)$$

(**F** being the total pinning force) since all vortices are initially subject to the same incremental shift dx. For sufficiently complete relaxation, we always obtain a pinning force equal to the derivative of the total potential energy $U(X)$ with respect to the c.m. position, X. We consider this to be a check of our numerical method.

In terms of the pinning strength A_p we observe three regions of qualitatively different types of behavior. For weak pinning strength $|A_p| \leq A_{el}$ (el designates the elastic instability) the distortion of the vortex lattice is elastic and reversible. All quantities vary smoothly and periodically as functions of the c.m. position with a period equal to the ideal lattice spacing, and thus the pinning force averaged over shift, $\bar{F}$, is zero. For somewhat stronger pins $A_{el} \leq |A_p| \leq A_{plas}$, we find a narrow region where the pins are strong enough to trap a vortex temporarily. As the strain builds up locally in the lattice around the trapped vortex, an elastic instability[4] occurs when the pinned vortex suddenly jumps off the pinning center and a new vortex jumps onto the pin. As a result of these instabilities $\bar{F}$ becomes finite in this region. The crossover value A_{el} decreases with increasing system size, approximately as the square root of the system size, and will eventually vanish for an infinite system.[5] This size dependence can be understood in terms of Larkin and Ovchinnikov's collective pinning theory if A_{el} is assumed to be equal to the pinning strength for which the size of a correlated lattice region becomes smaller than the system size.

For $|A_p| \geq A_{plas}$ the pins are sufficiently strong to trap individual vortices permanently, and plastic flow of the lattice around the fixed vortex becomes important. A_{plas} decreases weakly with increasing system size—our simulations are consistent with a $1/\log N_v$ dependence. The logarithmic decrease of A_{plas} is probably connected with the logarithmic decrease of the effective elastic constant describing the distortion of a finite 2D lattice due to a single pin. The characteristic features of this region are precipitous drops in the potential energy $U(X)$ (see Fig. 1), connected with a dramatic reordering of the vortex lattice. As the c.m. of the vortices is shifted, energy is pumped into the system, and the total potential energy increases approximately quadratically, with a corresponding linear increase in the force. Each of the linear sections of the force displacement curve $F(X)$ has, to a good approximation, the same slope and reaches the same maximum for a given set of control parameters and pin configuration. The energy is released when some of

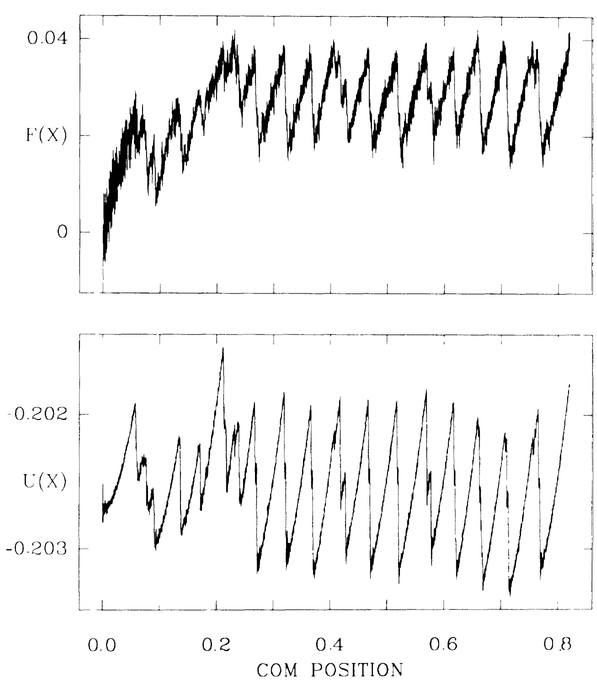

FIG. 1. The potential energy $U(X)$ and the pinning force $F(X)$ normalized by the number of vortices for the following set of parameters: $N_v = 340$, $R_v = 0.60$, $N_p = 146$, $A_p = -1.0$, and $R_p = 0.25$. The high-frequency noise is caused by the thermal fluctuations.

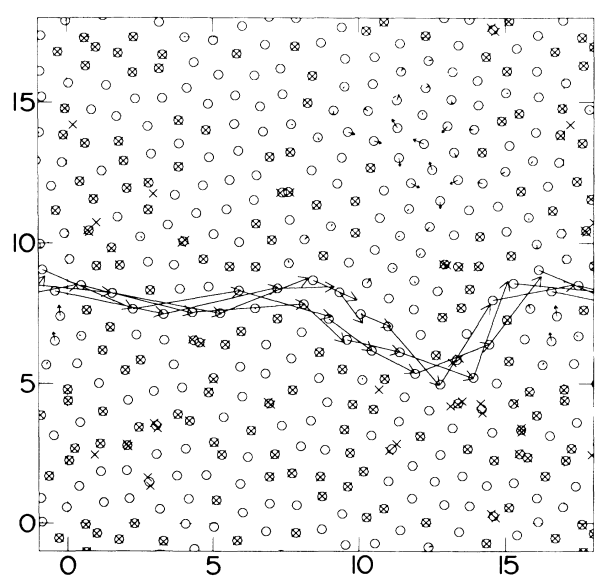

FIG. 2. Flow channels through the vortex lattice. Crosses are the fixed pins, circles are vortices. The arrows show how the vortices have moved while the c.m. has been shifted from $X = 0.24$ to 0.42. The configuration corresponds to the plots in Fig. 1.

the vortices suddenly start to flow plastically relative to the rest of the lattice (see Fig. 2). This flow takes place through *channel*-like paths, in between pinned regions of the lattice. The successive smooth increase and steep drop of the potential energy is associated with a reorganization of the vortices in the channels that has the form of a pulsating flow. The variation in $U(X)$ and $F(X)$ is repeated periodically with a periodicity specific to the given channels in operation. The periodicity changes if some channels close down and new ones start to flow. The periodicity typically corresponds to a shift of the c.m. of the order of $0.1a_0$, which leads to periods of the motion of the vortices in the channels of the order $[N_v/N_{v(\text{cha})}]0.1a_0$, where $N_{v(\text{cha})}$ is the number of vortices in the flowing channels. For pins somewhat stronger than the threshold A_{plas}, all or nearly all pins become saturated, each with one or more trapped vortices, and hence the other vortices see a set of fixed repulsive centers. For the higher pin densities this mechanism leads to *bottlenecks* in the channels, and the energy release is connected with a string of vortices hopping through a bottleneck. For lower densities of pins, the division of the vortices into nonmoving and moving is less sharp. The channels become broader with the largest movement taking place in the middle of the streams. In general the pinned areas remain trapped over the entire shift of the c.m..

It should also be noted that the sharp sawtoothed shape of $F(X)$ is obtained only if the lattice is relaxed sufficiently during the shift over the pins. Less complete relaxation gives us the same type of force displacement

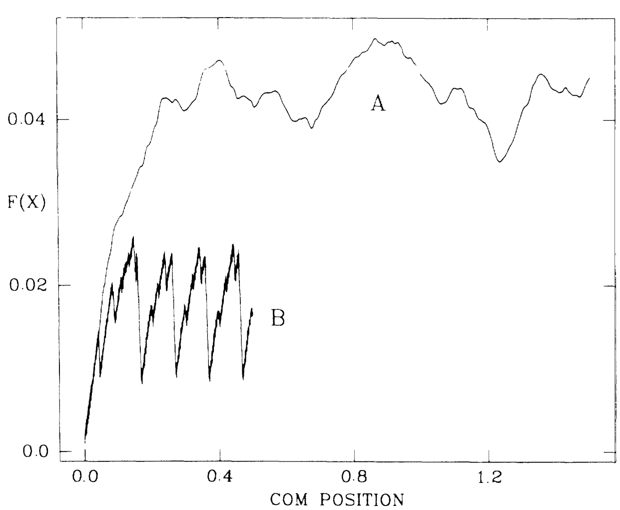

FIG. 3. The force-displacement curve $F(X)$ for two different degrees of relaxation for the same set of system parameters: $N_v = 340$, $R_v = 0.6$, $N_p = 105$, $A_p = -0.2$, and $R_p = 0.25$. Curve A was produced with an incremental shift $dx = 2\times10^{-4}$ and one relaxation per shift. For curve B $dx = 1\times10^{-4}$ and nine relaxations were made per shift. Curve B does not change upon further relaxation.

curves as obtained in Ref. 3. This is illustrated in Fig. 3 where $F(X)$ is shown for incompletely relaxed (curve A) and fully relaxed (curve B) simulations. Curve A is very similar to the result presented in Ref. 3 for the same parameters (but presumably for a different random placement of pins). Our criterion for complete relaxation, mentioned above, that $dU(X)/dX$ should equal the measured $F(X)$, is satisfied by the simulation which generated curve B but not for curve A.

We have analyzed the defects of the vortex lattice by calculating the root mean square deviation σ from the ideal lattice and the coordination number of all the vortices.[6] Defects in the vortex lattice show up as vortices with coordination numbers different from 6. For $|A_p| \le A_{\text{plas}}$ essentially no defects are observed whereas for $|A_p| \ge A_{\text{plas}}$ we always find a *highly* defective lattice. The total number of vortices with a specific coordination number varies, as the c.m. is shifted, in a complicated way. This is an indication of the delicate balance between storage of the lattice energy in the form of larger regions with pure elastic shear and storage of it in smaller sheared regions decoupled by lattice defects.

We consider the plastic flow through channels to be a qualitative feature of general importance to pinning of deformable lattices, especially to 2D pinning in type-II superconductors.[7] At least two important implications follow from this picture.

The first is in regard to the summation problem: The total pinning force may be considered to result from the combined effect of the pins in the flowing channels and the resistance to displacement of the vortices in the channels with respect to the pinned regions. The last term is determined by the flow stress of the lattice. As the pins become stronger, they eventually each trap a vortex, the channels narrow, and the pinning force saturates at a value given solely by the flow stress.[8] Collective pinning theory[1] is only applicable for pinning strengths $|A_p| \le A_{\text{plas}}$. We expect the region $|A_p| \ge A_{\text{plas}}$ to be the most relevant to flux pinning in macroscopic systems except for very weak-pinning superconductors in weak magnetic fields. We conjecture that the crossover away from collective pinning observed experimentally by Wördenweber, Kes, and Tseui[2] is caused by the onset of the channel flow described above.[9]

Second, the assumption that the flux motion takes place through a set of channels suggests that simple models can be used for analytic calculations of the dynamics of flux flow and also for the calculation of the noise spectrum associated with flux flow. This work is in progress.

One of us (H.J.J.) would like to thank E. H. Brandt for some very illuminating and clarifying discussions, and we wish to thank C. Kallin for stimulating discussions. One of us (H.J.J.) is partially supported by the Danish Natural Science Research Council, and another (A.B.) is the recipient of a NATO Fellowship. This work was supported by the Natural Sciences and Engineering Research Council of Canada.

[1]A. I. Larkin and Yu. N. Ovchinnikov, J. Low Temp. Phys. **34**, 409 (1979).

[2]R. Wördenweber, P. H. Kes, and C. C. Tsuei, Phys. Rev. B **33**, 3172 (1986); R. Wördenweber and P. H. Kes, Phys. Rev. B **34**, 494 (1986).

[3]E. H. Brandt, J. Low Temp. Phys. **53**, 41, 71 (1983), and Phys. Rev. Lett. **50**, 1599 (1983).

[4]See, L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon, New York, 1970), Sec. 21, for a discussion of elastic instabilities. This regime is "elastic" in the sense that the association of each particle with its neighbors in the flux lattice is unchanged by their motion through the random potential. By contrast, in the plastic regime, moving particles flow past neighbors which are pinned by the impurity potential.

[5]E. H. Brandt, Phys. Lett. **77A**, 484 (1980).

[6]J. P. McTague, D. Frenkel, and M. P. Allen, in *Ordering in Two Dimensions,* edited by S. K. Sinha (North-Holland, Amsterdam, 1980).

[7]Recently, A. Pruymboom, P. H. Kes, E. van der Drift, and S. Radellar (to be published) have performed experiments on channel flow in a type-II superconductor. It is also interesting to notice that this behavior was found in an analog experiment of the flux-line lattice. See P. H. Melville and M. T. Taylor, Cryogenics **10**, 491 (1970).

[8]R. Schmucker, Phys. Status Solidi (b) **80**, 8 (1977).

[9]At high fields the shear modulus C_{66} of the flux-line lattice in a type-II superconductor is known [see E. H. Brandt, Phys. Rev. B **34**, 6514 (1986)] to decrease as $(1-b)^2$, where $b=B/B_{c2}$ is the reduced field, B the internal field, and B_{c2} the upper critical field of the superconductor. Since the strength of the pinning potential decreases only as $1-b$ [see E. V. Thuneberg, J. Low Temp. Phys. **57**, 415 (1984)] the pinning centers become relatively stronger at high fields.