Molecular Dynamics Simulation on Vortex Lattice Melting in Meso-sopic Superconductors

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Abstract. Vortex lattice melting transitions in meso-sopic superconductors are studied using the molecular dynamics method for vortices. Temperature dependence of vortex dynamics comes from the fluctuation force and penetration dependence in the vortex-vortex interaction. Using the standard deviation of the positions of vortices, we can determine the melting temperature. Changing the vortex numbers, the melting temperature oscillates with increasing the vortex number.

1. Introduction
After the discovery of cuprate High-Tc superconductors [1], vortex states in the H-T phase diagram was explored in detail. The cuprate superconductors have many unconventional properties other than its higher transition temperature. Their Cooper pair symmetry is the d-wave and their conduction electron states are almost two dimensional and they have intrinsic Josephson junctions between superconducting layers. All of these properties are interesting and may useful for future applications. But also vortex states in the High-Tc cuprate superconductors are unique. In the pure High-Tc cuprate superconductor at low temperature and for higher field than lower critical field $H_{c1}$, vortices form a lattice. But for higher temperature this vortex lattice changes into a vortex liquid state [2]. There is a melting line of the vortex lattice. This melting behaviour comes from weak pinning, large thermal and quantum fluctuations in the cuprate High-Tc superconductors.

Recently, Ooi et al. showed the melting temperature in meso-sopic cuprate superconducting square plate oscillates with increasing magnetic field [3]. They explained this oscillation comes from the stability of configuration of $n^2$ vortices ($n=1,2,3,4,5,…$).

In order to confirm this phenomenon, we study the vortex lattice melting in meso-sopic superconductors using the molecular dynamics method for vortices [4,5]. Temperature dependence of vortex dynamics comes from the fluctuation force and penetration dependence in the vortex-vortex interaction. Using the standard deviation of the positions of vortices, we can determine the melting temperature. Changing the vortex numbers, we find the melting temperature depends on the vortex number.

In section 2, our method is explained and in section 3 we show numerical results. Section 4 is devoted to the summary.

2. Method
In the molecular dynamics method, a vortex are treated as a point-particle in a two dimensional space [3,4]. Previously we extended the molecular dynamics method including heat transport [5] and relaxation of superconducting order parameter [6]. In order to study the melting transition of a vortex lattice, we use a conventional molecular dynamics method because vortex motion is slow and heat generation and relaxation of order parameter are not important.

So, we solve following equation of motion for i-th vortex of which position is \( \mathbf{r}_i \).

\[
\eta \frac{d\mathbf{r}_i}{dt} = f_{\text{imp}}^{\text{imp}} + f_{\text{vi}} + f_{\text{vi}}
\]

(1)

Here \( \eta \) is the viscosity. The inertia term can be ignored comparing the viscosity term. The forces from pinning site is given as,

\[
f_{\text{imp}}^{\text{imp}} = \sum_j f_{\text{ij}}^p
\]

(2)

\[
f_{\text{ij}}^p = \frac{f_p}{r_p^3} \left( \frac{r_j - r^p_j}{\lambda} \right) \hat{r}_j
\]

(3)

where \( r^p_j \) is the position of j-th pinning site, \( \lambda \) is the penetration depth and \( f^p \) is the strength of the pinning force. The vortex-vortex interaction is given as,

\[
f_{\text{vi}} = \sum_j f_{\text{ij}}^{vv}
\]

(4)

\[
f_{\text{ij}}^{vv} = f_0 \sum_j K_1 \left( \frac{r_{ij}}{\lambda} \right) \hat{r}_j
\]

(5)

where \( f_0 = \Phi_0^2 / 8\pi^2\lambda^3 \) is the strength of the vortex-vortex and \( K_1(k) \) is the complete elliptic integral of the 1st kind. The thermal fluctuation force \( f_{\text{vi}} \) should satisfy following fluctuation-dissipation theorem,

\[
\langle f_{\text{vi}}(t_1) \cdot f_{\text{vi}}^*(t_2) \rangle = 2\eta k_B T \delta(t_1 - t_2)
\]

(6)

In this study, we consider mesoscopic superconducting square plate. Although the vortices are confined small superconducting plate, we use a periodic boundary condition. Temperature dependence of the vortex motion is taken into the penetration depth \( \lambda \) and the fluctuation force \( f_{\text{vi}} \).

3. Numerical Results

First we consider a small \((3\lambda \times 3\lambda)\) square superconducting plate, and put the fixed number of vortices randomly and then under the constant temperature we simulate the vortex motion using equation (1). In figure 1, we show the trajectories of vortices at the temperature \( T/T_c = 0.02 \). In this figure, each color of trajectories corresponds to each vortex. Because of the periodic boundary condition, trajectories of vortices are extended over the superconducting region \((3\lambda \times 3\lambda)\). From this figure, we can see all of the vortices remain in the small regions, which do not overlap with each other. Therefore this state can be considered as a solid of vortices.

Increasing the temperature, the motion of vortices becomes wild at \( T/T_c = 0.5 \) (figure 2). The vortex solid gradually melts. Further increasing the temperature, at \( T/T_c = 0.9 \), vortices move randomly over the superconducting region \((3\lambda \times 3\lambda)\), as shown in figure 3. In this state, now vortices become liquid.

In order to find the melting transition temperature, we calculate the variance of time averaged vortex positions.
Figure 1. Trajectories of 9 vortices in a $3\lambda \times 3\lambda$ square superconducting plate. Temperature is $T/T_c = 0.01$.

$$\sigma_i^2 = \left\langle \left( r_i - \langle r_i \rangle \right)^2 \right\rangle$$  \hspace{1cm} (7)

where average is taken over time interval from 0 to $t_{\text{TOTAL}}$. In this study, it happens that all of the vortices move to the same direction because of the periodic boundary condition, as seen in figure 2. In such case the variance of the vortex position becomes large, because the average of the position is the center of the trajectories in figure 2. But if we take the fixed boundary condition, the variance becomes rather small. In order to avoid this discrepancy, we divide the time interval into a series of short time intervals, calculate the variance for each short time interval and take average of the variances for all short time intervals. In figure 4, we show temperature dependence of the standard deviation $\sigma$, which is an average of the standard deviation $\sigma_i$ for 9 vortices. In this figure we see $\sigma$ abruptly becomes large around $T/T_c = 0.8$. This behavior corresponds to the vortex lattice melting.

Figure 2. Trajectories of 9 vortices in a $3\lambda \times 3\lambda$ square superconducting plate. Temperature is $T/T_c = 0.5$.

Figure 3. Trajectories of 9 vortices in a $3\lambda \times 3\lambda$ square superconducting plate. Temperature is $T/T_c = 0.9$. 
In figure 5, we show temperature dependences of the standard deviations for vortex number from 7 to 18. We can see that this temperature dependence does not monotonically depend on the vortex number.

![Figure 4](image)

**Figure 4.** Average of standard deviations of 9 vortices in the $3\lambda \times 3\lambda$ square superconducting plate as a function of temperature.

![Figure 5](image)

**Figure 5.** Average of standard deviations of vortices in the $3\lambda \times 3\lambda$ square superconducting plate as a function of temperature. Numbers of vortices are 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17 and 18.

4. Conclusion

In order to clarify the oscillation of the melting temperature as a function of the magnetic field in the meso-scopic superconducting square plate, numerical simulations of the molecular dynamics have been done. Temperature dependence is included in the penetration length and the fluctuation force in the simulation. Numerical results show that clear increase of the standard deviation of vortex positions with increasing the temperature. This increase means vortex lattice melting. We also have found that the standard deviation curves as a function of temperature show non-monotonic behavior, which may correspond to the oscillation behavior of the melting temperature as a function of the magnetic field in Reference [3].

In this study, we consider a model with the periodic boundary condition. But in the real system, vortices are confined in the finite region. So we will do similar simulations on a model with a fixed boundary condition including the effect of the Meissner current.
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