Vortex-lattice melting in magnesium diboride in terms of the elastic theory

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In the framework of elastic theory, we study the vortex-lattice melting transitions in magnesium diboride for magnetic fields both parallel and perpendicular to the anisotropy axis. Using the parameters from experiments, the vortex-lattice melting lines in the H-T diagram are located systematically by various groups of Lindemann numbers and the anisotropic parameters. It is observed that the theoretical result for the vortex melting with parallel and perpendicular fields agrees well with the experimental data.

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I. INTRODUCTION

Since the discovery of superconductivity with \( T_c = 39K \) in magnesium diboride (MgB2) was announced [1], it has caused a large number of experimental [2, 3, 4, 5, 6, 7, 8] and theoretical investigations [9, 10]. This introduced a new, simple (three atoms per unit cell) binary intermetallic superconductor with a record high (by nearly a factor of 2) superconducting transition temperature for a nonoxide and non-C60-based compound. It displays a variety of unusual properties. The high transition temperature seems to be either above or at the limit suggested theoretically several decades ago for BCS, phonon-mediated superconductivity [11]. It is characterized by a double band superconductor with two superconducting gaps of different size, the larger one originating from a quasi-2D \( \sigma \)-band and the smaller one from a 3D \( \pi \)-band. The electronic \( \sigma \)-states are confined to the boron planes and couple strongly to the in-plane vibration of the boron atoms. The unfixed anisotropic parameter \( \gamma \) vary widely, ranging from 1.1 to 6 depending on the measurement technique and on sample types [9, 12, 13, 14]. Although, some experimental data can shed light on the mechanism of superconductivity, it was demonstrated [13] that the type-II superconductivity may not be well described by the standard anisotropic Ginzburg-Landau theory, just due to the two-band structure.

The vortex-lattice solid (glass with random pinning) state with zero linear resistivity is crucial for the application of high-\( T_c \) superconductors, thus the melting of vortex-lattice in bulk type-II superconductors is of great significance [16, 17, 18, 19, 20]. The traditional Lindemann theory suggests that the lattice melts when the root mean square thermal displacements of the components of a lattice reach a certain fraction of the equilibrium lattice spacing. This criterion was first adopted to study the vortex-lattice melting transition in type-II superconductors with a magnetic field parallel to the anisotropic axis [17], then it was used to draw the melting lines when magnetic field is perpendicular to the anisotropic axis [21, 22, 23, 24]. Since the upper critical field is also high in MgB2, the thermal fluctuation may drive the vortex-lattice to a vortex liquid in a field far below the upper critical field [21] through vortex melting.

In this paper, using the parameters measured in recent two typical experiments [7, 8], we study the vortex-lattice melting transitions in the framework of the elastic theory phenomenologically. The melting lines for magnetic fields both parallel and perpendicular to the anisotropic axis are systematically located with different groups of Lindemann numbers and anisotropic parameter. The comparison with experiments are also made. The present paper is organized as follows. In Section 2, we introduce the theoretical method. Section 3 presents the main results. We give a short summary in the final section.

II. ELASTIC THEORY

For ideal triangular vortex-line lattice, the free energy in elastic theory for fields parallel and perpendicular to the \( x \) axis can be generally written with quadratic terms of the deviation vector \( \mathbf{u} = (u_x, u_y) \) describing the fluctuations of vortices from their equilibrium positions [16, 17, 21, 22, 23, 24, 25]

\[
F = \frac{1}{2} \int \frac{d^2k}{(2\pi)^2} \mathbf{u} \cdot \mathbf{C} \cdot \mathbf{u},
\]

(1)

The matrix \( \mathbf{C} \) for parallel fields is different from that for perpendicular fields. We denote \( \mathbf{C}^c \) and \( \mathbf{C}^{ab} \) to be the elastic matrix for the fields parallel and perpendicular to \( c \)-axis, respectively, which are given as follows

\[
\mathbf{C}^c = \begin{pmatrix}
    c_{11}k_x^2 + c_{66}k_1^2 + c_{44}k_2^2 & c_{12}k_xk_y \\
    c_{12}k_xk_y & c_{22}k_y^2 + c_{66}k_1^2 + c_{44}k_2^2
\end{pmatrix}
\]

(2)

and

\[
\mathbf{C}^{ab} = \begin{pmatrix}
    c_{11}k_x^2 + c_{66}k_1^2 + c_{44}k_2^2 & c_{12}k_xk_y \\
    c_{12}k_xk_y & c_{22}k_y^2 + c_{66}k_1^2 + c_{44}k_2^2
\end{pmatrix}
\]

(3)

where

\[
\mathbf{u}_c = \begin{pmatrix}
    u_x \\
    u_y
\end{pmatrix}, \quad \mathbf{u}^{ab} = \begin{pmatrix}
    u_x \\
    u_y
\end{pmatrix}
\]
where $k_x^2 = k_x^2 + k_y^2$, $c_{66}, c_{L} = c_{11} - c_{66}$, and $c_{44}$ are the wave-vector-dependent shear, bulk, and tilt elastic moduli. The detailed expressions for these moduli can be found in several previous papers [16, 17, 22, 24, 25]. The thermal fluctuations of the vortices are given by inverting

$$\langle u^2 \rangle = \frac{k_B T}{2\pi^2} \int d\mathbf{k} |\mathbf{C}^{3 \alpha \beta}(\mathbf{k})|^{-1}, \alpha = x, y, \beta = c, ab. \hspace{1cm} (4)$$

The Lindemann criterion presumes that the lattice melts, when the root mean square thermal displacements of the components of a lattice reach some fraction of the equilibrium lattice spacing. For parallel fields, we consider the mean-square displacement of a vortex lattice from the equilibrium $d^2(T) = u_x^2 + u_y^2$, then use the usual isotropic Lindemann criterion,

$$\langle d^2 \rangle = c^2 a^2. \hspace{1cm} (5)$$

For perpendicular fields, an anisotropic Lindemann criterion should be employed

$$\langle u_x^2 \rangle = c_x^2 a_x^2, \hspace{0.5cm} \langle u_y^2 \rangle = c_y^2 a_y^2. \hspace{1cm} (6)$$

with $c_x$ and $c_y$ are two Lindemann numbers for two transverse directions. Combining the Lindemann criterion and the elastic theory, the melting equations are derived with the Lindemann coefficients $c'$s.

If fields are applied perpendicular to c-axis, the effect of layer pinning reduces fluctuations in both directions and induces an additional momentum-independent term to the elastic matrix in Eq. (3) such that

$$\mathbf{C}_{lp}^{ab} = \left( \begin{array}{cccc} c_{11}k_x^2 + \frac{c_{12}h_y^2}{c_{66}k_y^2} & \frac{c_{11}k_xk_y}{c_{66}k_y} & \frac{c_{11}k_xk_y}{c_{44}k_y^2} & \frac{c_{11}k_xk_y}{c_{66}k_y} \\ \frac{c_{11}k_xk_y}{c_{66}k_y} & c_{11}k_y^2 + \frac{c_{12}h_x^2}{c_{66}k_x^2} & \frac{c_{11}k_xk_y}{c_{44}k_x^2} & \frac{c_{11}k_xk_y}{c_{66}k_x^2} \\ \frac{c_{11}k_xk_y}{c_{66}k_y} & \frac{c_{11}k_xk_y}{c_{66}k_y} & c_{11}k_y^2 + \frac{c_{12}h_x^2}{c_{66}k_x^2} & \frac{c_{11}k_xk_y}{c_{44}k_x^2} \\ \frac{c_{11}k_xk_y}{c_{66}k_y} & \frac{c_{11}k_xk_y}{c_{66}k_y} & \frac{c_{11}k_xk_y}{c_{66}k_y} & c_{11}k_y^2 + \frac{c_{12}h_x^2}{c_{66}k_x^2} \end{array} \right)$$

where $\Theta$ is proportional to the critical depinning current and depends on the layer separation $s$ [28].

III. RESULTS AND DISCUSSIONS

A. Vortex melting lines for fields parallel to the c-axis

First, we calculate the melting line of MgB$_2$ thin film for fields parallel to the c-axis. The experiments were performed by Wen et al. [7]. We employ the experimental parameters as follows: the zero-field superconducting transition temperature $T_c = 39 \text{K}$, the Ginzburg-Landau parameters $\kappa = 26$, the upper critical fields along c axis $H_{c2}^0(T = 0) = 15.7 \text{Tesla}$. Since the anisotropy coefficient $\gamma = \frac{H_{c2}^0}{H_{c2}^0}$, is not well established for MgB$_2$, [12, 13, 14] we vary the anisotropic parameter $\gamma$ in the range of 1.5 to 4.5 in our calculation. When fields parallel to the c-axis, we set $c_x = c_y = 0.1$ and with the variation of $\gamma$, as shown in Fig.1. Interesting, in the inset of Fig.1 we find that the melting line with $\gamma = 3$ agrees well with the irreversibility lines measured by SQUID in ref. [7]. The irreversibility line in superconductor is usually regarded as the melting line. [21]. The value of $\gamma = 3$ in this sample is similar to that on transport measurements of the upper critical field anisotropy performed on single crystals [12, 14].

Then, we evaluate the melting line of MgB$_2$ single crystal for fields parallel to the c-axis. This experiment
was done by Eltsev et al. [8]. The experimental parameters measured from Ref. [8] are collected as follows: $T_c = 38.5\,\text{K}$, $\kappa = 26$, $H_{c2}^\text{tot}(T = 0) = 7.5\,T$. We also change the anisotropic parameter $\gamma$ from 1.5 to 4.5 as above. It is found that the variation of $\gamma$ also has influence on the melting line. Fig. 2 shows the theoretical melting results with $c_x = c_y = 0.1$, where the experimental data are also exhibited. As shown in the inset of Fig. 2, we observe that the melting line with $\gamma = 3$ agrees with experimental data [8]. Here the resulted anisotropic parameter $\gamma = 3$ also matches up to the experiment results on transport measurements of $MgB_2$ single crystals [12, 14].

### B. Vortex melting lines for fields perpendicular to the $c$-axis

We next turn to the vortex melting transition for fields perpendicular to $c$-axis. The experimental parameters for a $MgB_2$ single crystal are taken from Ref. [8] as the following: $T_c = 38.5\,\text{K}$, $\gamma = 3$, $\kappa = 26$, $H_{c2}^\text{tot}(T = 0) = 22T$. Following the procedure outlined in the preceding section, we calculate the thermal fluctuations in the two transverse directions. Setting $C_x = C_y = 0.14$, we obtain two curves similar to those in Ref. [22], which are shown in Fig. 3. As pointed out in Ref. [22], to interpret these two curves as two "melting lines" and thus reach to a conclusion of an intermediate smectic phase is unphysical, since the elastic theory can give at best one single melting line. To impose the same Lindemann number along the two directions is of no physical basis. In order to achieve a single melting line, we tune the Lindemann number $c_y$ at 0.1. A good collapse of the melting lines in two directions can be achieved if setting the ratio $c_x/c_y \approx 1.4$, as shown in Fig. 3. It is interesting to note that this ratio is very close to 1.37 observed in Ref. [24] using parameters in cuprate superconductors. More importantly, we reproduce reasonably the experimental melting line in Ref. [8] as shown in fig. 3.

The vortex melting for fields perpendicular to the $c$-axis is also influenced by the layer pinning. In order to study this intrinsic layer pinning effect, the matrix (7) is used to calculate the thermal fluctuations along two transverse directions. Here, the layer separation of magnesium diboride is $s = 3.524\,\text{Å}$ [1]. The melting lines for $\gamma = 3$ with Lindemann number $c_x = c_y = 0.12$ are collected in Fig. 4. We find that the melting line with $c_x = 0.12$ matches the experimental data. By tuning the Lindemann number $c_y$, a good collapse can also be obtained by setting the same ration $c_x/c_y \approx 1.33$.

### IV. SUMMARY

In the framework of the elastic theory, we have studied the melting transition in magnesium diboride for magnetic fields parallel and perpendicular to the anisotropy axis. Using the parameters from experiments, the melting lines with various Lindemann numbers and the anisotropic parameter are composed. Although the anisotropic parameter varies with the different measurement technique and sample types, the melting lines derived here agree well with those in thin films [5] and single crystal [8] by using Lindemann number $c_x = 0.1$ and anisotropic parameter $\gamma = 3$ for magnetic field parallel to the $c$–axis. For fields perpendicular to the $c$-axis, it is observed that thermal fluctuations normalized by vortex separations in the two transverse directions are proportional to each other, similar to those observed in cuprate superconductors. The ratio $c_x/c_y$ to achieve a single melting line is very close to that observed in Ref. [24]. More interestingly, by using $c_x = 0.12$ and $c_y = 0.09$, we are able to draw the melting line which fits the experimental melting line in [8] quite well. Although the standard anisotropic Ginzburg-Landau theory may not be applicable to magnesium diboride, the elastic theory of vortex matter can provide a good description of the vortex melting in this two-band superconductors.
Acknowledgments

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