Properties of parallel upper critical field within Continuous Ginzburg-Landau model

L. Wang, H. S. Lim, and C. K. Ong
Center for Superconducting and Magnetic Materials and Department of Physics, Blk. S12, Faculty of Science, National University of Singapore, 2 Science Drive 3, Singapore 117542.

In this paper, we employ a continuous Ginzburg-Landau model to study the behaviors of the parallel upper critical field of an intrinsically-layered superconductor. Near $T_c$ where the order parameter is nearly homogeneous, the parallel upper critical field is found to vary as $(1 - T/T_c)^{1/2}$. With a well-localized order parameter, the same field temperature dependence holds over the whole temperature range. The profile of the order parameter at the parallel upper critical field may be of a Gaussian type, which is consistent with the usual linear Ginzburg-Landau theory. In addition, the influences of the unit cell dimension and the average effective masses on the parallel upper critical field and the associated order parameter are also addressed.

I. INTRODUCTION

Most high $T_c$ superconductors (HTSs) have layered structures and the layered superconductivity is closely related to the behavior of the order parameter. Spatial variation of the order parameter would aid us to intuitively understand various properties such as the coherence lengths of layered superconductors. On the other hand, the investigation of the upper critical field $B_{c2}$ may provide information on the coherence lengths, and in principle, allow the testing of existing theories (for example, see Refs. 1–7). Hence, a study involving the order parameter and the upper critical field should prove valuable.

The phenomenological continuous Ginzburg-Landau (CGL) model is convenient for a description of the order parameter and the upper critical field of layered superconductors. The coefficients in the CGL free energy are assumed to be spatially dependent. As a result, the amplitude of the order parameter varies, reflecting the layered nature. The amplitude of the order parameter at weakly superconducting layers may be extremely small, corresponding to a weakly linked layer system similar to the Lawrence-Doniach (LD) model. On the other hand, when the spatial dependence is neglected, the CGL model is reduced to the anisotropic Ginzburg-Landau (GL) model. Hence, the CGL model approaches the limiting cases of the LD model and the anisotropic GL model.

In a previous work, a set of spatial coefficients for the CGL model was proposed for a layered superconducting system in which the unit cell was assumed to compose of equivalently thick superconducting and insulating layers and no applied magnetic field was present. Recently, a magnetic field parallel to the layers with different thickness was introduced and efficient computing methods have been adopted to determine the generic properties of the parallel upper critical field $B_{c2}^{||}$ of various layered superconductors. In the present work, we shall examine various features pertinent to $B_{c2}^{||}$ and the associated order parameter of a typically-layered superconductor.

II. MODEL

In the CGL model of Koyama et al. layered superconductors have been classified into three categories, one of which the layered HTS Bi$_2$Sr$_2$CaCu$_2$O$_{8}$ (Bi2212) may fall into. Following Ref. 8, Bi2212 shall be chosen as our modeling prototype for layered superconductors as it possesses a large anisotropy, and thus is suitable for a detailed study that examines the relationship between the amplitude of the order parameter and the layered structure. Note, however, that a study involving the phase effect of the order parameter (Josephson coupling) in Bi2212 may require a LD description for an appropriate investigation.

The unit cell of Bi2212 comprises of two CuO$_2$ bilayers, separated by the BiO-SrO interlayer, which is referred to as insulating (I) layer for convenience. The two adjacent CuO$_2$ planes of the bilayer (interplane distance $\sim$ 3 Å) are strongly coupled so that they can be treated as a single superconducting (S) layer; therefore the distance between two superconducting layers is half the c-axis lattice constant $\sim$ 15 Å. Denoting the thickness of the I and S layers as $d_I$ and $d_S$, respectively, we may write the size of the unit cell $D$ as $D = d_I + d_S$. The CGL free energy for the system is

$$ F = \int dV \left[ \alpha(T, z)|\Psi(\vec{r}, z)|^2 + \frac{1}{2} \beta |\Psi(\vec{r}, z)|^4 + \frac{\hbar^2}{2M(z)} \left( \frac{\partial}{\partial z} - \frac{2ie}{\hbar} A_z(\vec{r}, z) \right) \Psi(\vec{r}, z) \right]^2 $$
with planar vector \( \vec{r} = (x, y) \) and vector potential \( \vec{A}(\vec{r}, z) = (\vec{A}(z)(\vec{r}, z), A_z(\vec{r}, z)) \). \( M(z) \) denotes the effective masses along the \( z \)-direction (\( c \)-axis), and \( m(z) \) is the corresponding planar parameter. The GL coefficient \( \alpha(T, z) \) and the effective masses are taken as before \((\beta \) is assumed as a constant):\[\begin{align*}
\alpha(T, z) &= [\alpha_0 + \alpha_1 \cos(2\pi z/D)](1 - T/T_c), \\
\frac{1}{M(z)} &= G_0 + G_1 \cos(2\pi z/D), \\
\frac{1}{m(z)} &= g_0 + g_1 \cos(2\pi z/D),
\end{align*}\]

For a given temperature \( T \), the maximum magnetic field \( B \) which satisfies the above equation, together with the boundary conditions \( \Psi(0) = \Psi(D) \) and \( \frac{\partial}{\partial z} \Psi(z)|_{z=0} = 0 \), gives a point on the \( B_{c2}(T) \) curve. The largest \( B \) can be readily achieved by treating \( B^2 \) in Eq. 4 as eigenvalue problem.\[\begin{align*}
\frac{\hbar^2}{2m(z)} \frac{\partial^2}{\partial z^2} \Psi(z) - \frac{\hbar^2}{2} \left[ \frac{\partial}{\partial z} \frac{1}{M(z)} \right] \frac{\partial}{\partial z} \Psi(z) + \\
\frac{1}{2m(z)} (2eB)^2(z - z_0)^2 + \frac{\hbar^2 k_y^2}{2m(z)} \Psi(z) + \\
\alpha(T, z) \Psi(z) + \beta |\Psi(z)|^2 \Psi(z) = 0,
\end{align*}\]

with \( z_0 = \hbar k_y/(2eB) \). At \( B = B_{c2} \), the superconducting order develops in the \( S \) layer first so that one may choose \( z_0 = D/2 \). The high order term in Eq. 3, \( \beta |\Psi(z)|^2 \Psi(z) \), may be omitted since the order parameter at \( B_{c2} \) is physically small. To explore the features of the order parameter along the \( z \) direction, we assume \( k_y = 0 \). Finally, we obtain

\[\begin{align*}
\frac{\hbar^2}{2m(z)} \frac{\partial^2}{\partial z^2} \Psi(z) - \frac{\hbar^2}{2} \left[ \frac{\partial}{\partial z} \frac{1}{M(z)} \right] \frac{\partial}{\partial z} \Psi(z) + \\
\frac{1}{2m(z)} (2eB)^2(z - z_0)^2 + \frac{\hbar^2 k_y^2}{2m(z)} \Psi(z) + \\
\alpha(T, z) \Psi(z) + \beta |\Psi(z)|^2 \Psi(z) = 0,
\end{align*}\]

III. RESULTS AND DISCUSSION

The order parameter distribution in a unit cell at different temperatures is plotted in Fig. 1(a). At low temperatures, the order parameter is mainly confined within the \( S \) layer, signifying a two-dimensional (2-D) state. At high temperatures, it effectively penetrates into the \( I \) layers. Near \( T_c \), it varies smoothly and is nearly a constant throughout the unit cell, indicating a three-dimensional (3-D) state behavior. The present model thus correctly accounts for the behavior of a 2-D state at lower temperatures and a 3-D state near \( T_c \). Note that the weak modulation of the order parameter near \( T_c \) may generate a genuine 3-D superconductor. This is different from the so-called 3-D region of the LD model, where the interlayer coherence length is much larger than the interlayer spacing or the size of the unit cell, but the order parameter is still assumed to be discontinuous. Thus, there is the possibility of a true 3-D superconductivity with a nearly uniformly distributed order parameter even in a highly anisotropic superconductor. This situation can be obtained by just varying the temperature (see Fig. 1(a)).

Again, it is found that the peaks of the order parameter can be fitted by a Gaussian function. The exponential factor is the most significant part of the Gaussian fit, showing that the ground state of the CGL linear equation is similar to that of the usual linear GL equation. We emphasize that this similarity, together with many reasonable results to be presented, reveals the plausibility of our methods of calculating \( B_{c2} \). The fitted \( \xi(0) \) is 0.96 \( \AA \), which compares favorably with some experimental values of \( \sim 1 \ \AA \).

The calculated parallel \( B_{c2} \) as a function of temperature is shown in Fig. 1(b) and Fig. 2. Near \( T_c \), the feature of \( B_{c2}(T) \) is square-root like while far away from \( T_c \), it is linear. The linear behavior in Fig. 1(b) can be understood by identifying \( B_{c2} \propto 1/\xi^2 \) while the latter is proportional to \( 1 - T/T_c \). Note that the relationship between \( B_{c2} \) and \( T \) is also linear within the
anisotropy GL theory, in which $B_{c2}(T) = \frac{\Phi_0}{2\pi c(T)\xi_\perp(T)}$, where both the interlayer and in-plane coherence lengths $\xi_\perp(T)$ and $\xi_\parallel(T)$ are proportional to $(1 - T/T_c)^{-1/2}$ so that $B_{c2}(T) \propto (1 - T/T_c)$.

Since the parallel $B_{c2}$ in Bi2212 rapidly exceeds accessible laboratory magnetic fields when the temperature is reduced from $T_c$, only the calculated data near $T_c$ can be compared with experiments (see Fig. 2). By considering a constant solution of the order parameter to Eq. 4, one can immediately obtain a square-root $B_{c2}$-T relation near $T_c$. Note, however, that with open boundary conditions (OBC, $\Psi(z)|_{z=\pm\infty} = 0$) imposed on Eq. 4, we have found that there is a linear $B_{c2}$-T relation near $T_c$ (see solid circles in Fig. 2). The deviation from the linear behavior can be understood as a dimensional crossover (see solid circles in Fig. 2). The deviation from the linear behavior near $T_c$ indicates that the upward curvature of the $B_{c2}$-T curve is absent in the present simulated system. Recent studies show that the upward curvature is perhaps not intrinsic. Indeed, such curves are neither found nor obvious in the WHH approximation, the d-wave theory and the mixed d- and s-wave theory. Note, however, that the feature of the $B_{c2}$-T curvature is controversial and remains to be tested. According to Fig. 2, the curvature of $B_{c2}$-T is boundary-condition dependent and thus indeed difficult to arrive at an absolutely conclusive conclusion. The curvature may also be affected by physical phenomena such as the spin orbit scattering (for example, see the microscopic theory in Ref. 2).

The calculated $B_{c2}$ at zero temperature is about 700 Tesla and is comparable with those extrapolated from experiments on Bi2212 and other HTS such as YBCO and Bi2Sr2Ca2Cu3O10. However, the experimentally extrapolated data might not be too reliable and a possible new way to detect $B_{c2}$ with Josephson plasma has been suggested.

Fig. 3(a) shows the spatial distribution of the order parameter for different $D$ of the unit cell at zero temperature. For small $D$, the order parameter covers the entire I layer but as $D$ increases, its penetrations into the neighboring I layers become restricted and quickly fall to zero. The 3-D (2-D) behavior for small (large) unit cell is in accordance with the features reflected in the calculated $B_{c2}$-T curves of Refs. 2. Fig. 3(b) presents the variation of the upper critical field with the size of the unit cell at $T = 0 \ K$. The obtained critical field decreases with $D$, which is qualitatively consistent with the $g_3$ model. Here a power law (dash line) could not fit the trend well but an exponential fit (solid line) is acceptable. Experimentally, for the similar compounds of Tl2Ba2Ca$_{n-1}$Cu$_n$O$_{2n+4}$ ($n=1,2,4$), Mukaida et al. reported that the upper critical field generally decreases as the number of CuO$_2$ layer increases. They attributed their results to the effects caused by the different thickness of the effective superconducting layers in Tl$_2$Ba$_2$CuO$_6$, Tl$_2$Ba$_2$CaCu$_2$O$_8$ and Tl$_2$Ba$_2$Ca$_3$Cu$_4$O$_{12}$, whose respective c-axis lattice constants are 23.2, 29.3 and 41.9 A. Clearly, the theoretical trend presented in Fig. 3(b) is consistent with their experimental observations.

The mass dependences of the parallel upper critical field at zero temperature are shown in Fig. 4(a) and (b). In these calculations, the value of $G_1 (g_1)$ was fixed while that of $G_0 (g_0)$ was varied to obtain the varying $M_\perp (m_\perp)$. It is clear that large values of both $M_\perp$ and $m_\perp$ result in a large critical field, which is consistent with the anisotropic GL theory, the LD model and the $g_3$ theory. It is worth mentioning that as $M_\perp$ increases, we find that the order parameter $\Psi(D/2)$ at the S layer grows while that at the I layer, $\Psi(0)$, decreases, leading to a larger difference of $\Psi(D/2) - \Psi(0)$. Since $(\Psi(D/2) - \Psi(0))$ is approximately proportional to the strength of interlayer coupling between adjacent S and I layers; thus $M_\perp$ suppresses interlayer coupling. In contrast, $m_\parallel$ is found to enhance interlayer coupling. We attribute this to the effect that $M_\perp$ enhances the order parameter in the superconducting layer while $m_\parallel$ suppresses it. Hence, HTS are intrinsically favorable for a large $M_\perp$, which corresponds to a weakly linked layered system.

The spatial variation of the order parameter at several condensation energies is plotted in Fig. 5(a). The temperature is set to zero. It is obvious that the largest energy corresponds to the largest order parameter in the S layer and that the smaller the condensed energy, the broader the order parameter. Fig. 5(b) further shows that the critical field increases with the condensation energy.

Up till now, we have set the parameters $a_0$, $a_1$, $G_0$, $G_1$, $g_0$ and $g_1$ (see Eq. 2) in the S layer the same as those in the I layer (for example, $a_0^S = a_0^I$). We shall now consider the case where $a_0^S \neq a_0^I$. The ratios of $a_0^S/a_0^I$ in Fig. 6 (a) and (b) are 20 and 2000000, respectively. The temperature is zero. The non-monotonic trend (first ascending and then descending) in Fig. 6(a) is qualitatively consistent with the data extracted from the numerical work of Refs. 2.

When the energy condensed in the S layer is extremely large, the system would be in an extreme 2-D state, as illustrated in Fig. 6(b) for different unit cell sizes. The order parameter totally resides in the S layer. The S layer fully decouples with the adjacent I layers and therefore the system is in an extreme 2-D state. This interesting 2-D behavior can be confirmed by the thickness dependence of the upper critical field. The theoretical data can be fitted by an inverse relation typical of a 2-D system (for example, see Refs. 2). It is interesting to find that the $\Psi(D/2)$-D profile is qualitatively consistent with the $B_{c2}$-D trend. Such qualitative consistency can also be
found in Figs. 6(a) and 3.

The extreme 2-D behavior can be further confirmed by the spatial distribution of the order parameter and the temperature dependence of the upper critical field, which are shown in Fig. 7. In Fig. 7 (a), the order parameter drops down sharply and is confined in the S layer in a large temperature range till 84.9 K. In Fig. 7 (b), a square-root relation between $B_{c2}$ and $T$ holds over the whole temperature range and this again is a typical 2-D behavior, which has been reported in the literature (for example, see Refs. [3] and [4]).

IV. CONCLUSION

Within a continuous Ginzburg-Landau model for layered superconductors, we have calculated the parallel upper critical field and the associated order parameter with respect to the variation of the temperature, the unit cell dimension, the average effective masses and the GL condensation energy. Near the vicinity of $T_c$ where the order parameter is nearly homogeneous, the parallel upper critical field is found to be square-root like. With a highly localized superconductivity, the same field temperature dependence holds over the whole temperature range. The order parameter at $B_{c2}$ of the linear CGL equation may demonstrate a Gaussian profile, which is consistent with that of the usual linear GL equation. The profile of the maximum order parameter in the superconducting layer against the unit cell size may be correlated with the trend of the upper critical field versus the unit cell dimension.

1. W. E. Lawrence and S. Doniach, Proc. 12th Int. Conf. on Low Temp. Phys., edited by E. Kanda (Academic Press of Japan, Kyoto, 1971), p. 361.
2. R. A. Klemm, A. Luther, and M. R. Beasley, Phys. Rev. B 12, 877 (1975).
3. S. Takahashi and M. Tachiki, Phys. Rev. B 33, 4620 (1986); M. Tachiki and S. Takahashi, Physica C 153-155, 1702 (1988).
4. T. Koyama, N. Takezawa, Y. Naruse, and M. Tachiki, Physica C 194, 20 (1992).
5. T. Schneider and A. Schmidt, Phys. Rev. B 47, 5915 (1993).
6. V. B. Geshkenbein, L. B. Ioffe, and A. J. Millis, Phys. Rev. Lett. 80, 5778 (1998).
7. Yu. N. Ovchinnikov and V. Z. Kresin, Phys. Rev. B 52, 3075 (1995); G. Kotliar and C. M. Varma, Phys. Rev. Lett. 77, 2296 (1996); A. A. Abrikosov, Phys. Rev. B 56, 446 (1997); A. S. Alexandrov, W. H. Beere, V. V. Kabanov, and W. Y. Liang, Phys. Rev. Lett. 79, 1551 (1997).
8. L. Wang, H. S. Lim, and C. K. Ong, Supercond. Sci. Technol. 14, 252 (2001).
9. L. Wang, H. S. Lim, and C. K. Ong, accepted for publication in Supercond. Sci. Technol. (2001).
10. N. Takezawa, T. Koyama, and M. Tachiki, Physica C 207, 231 (1993).
11. D. E. Farrell, S. Bonham, J. Foster, Y. C. Chang, P. Z. Jiang, K. G. Vandervoort, D. J. Lam, and V. G. Kogan, Phys. Rev. Lett. 63, 782 (1989).
12. R. Kleiner, F. Steinmeyer, G. Kunkel, and P. Müller, Phys. Rev. Lett. 68, 2394 (1992); R. Kleiner and P. Müller, Phys. Rev. B 49, 1327 (1994).
13. J. M. Tarason, Y. Le Page, P. Barboux, B. G. Bagley, L. H. Greene, W. R. Mckinnon, G. W. Hull, M. Giroud, and D. M. Hwang, Phys. Rev. B 37, 9382 (1988).
14. A. A. Abrikosov, Zh. Eksp. Teor. Fiz. 32, 1442 (1957) [Sov. Phys. JETP 5, 1174 (1957)].
15. M. Tinkham, Introduction to Superconductivity (McGraw-Hill, New York, 1996).
16. S. H. Han, Y. Eiltsev, and Ö. Rapp, Phys. Rev. B 57, 7510 (1998); Y. Hidaka, M. Oda, M. Suzuki, Y. Maeda, Y. Enomoto, and T. Murakami, Jpn. J. Appl. Phys. 27, L538 (1988). Note, however, that there are discrepancies among the values of $\xi_c(0)$ for Bi2212, see, A. Pomar, M. V. Ramallo, J. Mosquera, C. Torrón, and F. Vidal, Phys. Rev. B 54, 7470 (1996).
17. T. T. M. Palstra, B. Batlogg, L. F. Schneemeyer, R. B. van Dover, and J. V. Waszczak, Phys. Rev. B 38, 5102 (1988).
18. Y. Koike, T. Nakamoto, and T. Fukase, Jpn. J. Appl. Phys. 27, L841 (1988).
19. Cornell S. L. Chun, Guo-Guang Zheng, Jose L. Vicent, and Ivan K. Schuller, Phys. Rev. B 29, 4915 (1984).
20. H. H. Wen, W. L. Yang, Z. X. Zhao, and Y. M. Ni, Phys. Rev. Lett. 82, 410 (1999).
21. N. R. Werthamer, E. Helfand, and P. C. Hohenberg, Phys. Rev. 147, 295 (1966).
22. H. Won and K. Maki, Phys. Rev. B 53, 5927 (1996).
23. W. Kim, J. X. Zhu, and C. S. Ting, Phys. Rev. B 58, 607 (1998).
24. M. C. Dai, T. J. Yang, and C. S. Ting, Phys. Rev. B 59, 9508 (1999).
25. C. Uher, J. L. Cohn, and Ivan K. Schuller, Phys. Rev. B 34, 4906 (1986).
26. U. Welp, W. K. Kwok, G. W. Crabtree, K. G. Vandervoort, and J. Z. Liu, Phys. Rev. Lett. 62, 1908 (1989).
27. I. Matsubara, H. Tanigawa, T. Ogura, H. Yamashita, M. Kinoshita, and T. Kawai, Phys. Rev. B 45, 7414 (1992).
28. M. C. de Andrade, Y. Dalichaouch, and M. B. Maple, Phys. Rev. 48, 16737 (1993).
29. A. A. Abrikosov, Phys. Rev. B 38, 5112 (1997).
30. H. Mukaida, K. Kawaguchi, M. Nakao, H. Kumakura, D. R. Dieterich, and K. Togano, Phys. Rev. B 42, 2659 (1990).
31. V. G. Kogan, Phys. Rev. B 24, 1572 (1981); V. G. Kogan and J. R. Clem, Phys. Rev. B 24, 2497 (1981).
32. V. I. Dediu, V. V. Kabanov, and A. S. Sidorenko, Phys. Rev. B 49, 4027 (1994).
33. A. Sidorenko, C. Sütgers, T. Trappmann, and H. v. Löhneysen, Phys. Rev. B 53, 11751 (1996).

FIG. 1. (a) Spatial distribution of the order parameter for different temperatures. (b) Temperature dependence of the parallel upper critical field.
FIG. 2. Calculated temperature dependences of the parallel upper critical field near $T_c$, compared with experiments. The solid squares correspond to the periodic boundary condition with spatial-dependent coefficients (CGL), the solid circles to the open boundary conditions with spatial-dependent coefficients (CGL) and the open diamonds to the open boundary conditions with spatial-independent coefficients (AGL). The solid line is a fit varying as $(1 - T/T_c)^{0.5}$. The dotted line signifies the crossover temperature from 3D to 2D in the PBC-CGL (solid squares) and OBC-CGL (solid circles) calculations.

FIG. 3. (a) Order parameter distribution and (b) upper critical field at different sizes of the unit cell.

FIG. 4. Upper critical field for (a) perpendicular average mass $M_\perp$ and (b) parallel average mass $m_\parallel$.

FIG. 5. a) Order parameter distribution and (b) upper critical field at different condensation energies.

FIG. 6. Order parameter and upper critical field for $\alpha_0^S/\alpha_0^I = 20$ in (a) and $\alpha_0^S/\alpha_0^I = 2000000$ in (b). The profiles of the maximum order parameter vs $D$ seem consistent with the corresponding $B_{c2}-D$ trends. The dash line in (b) is approximately an inverse fit while the solid line is an exponential decay.

FIG. 7. Typical 2D temperature dependence of the parallel upper critical field.
Figure 2

- calc. (PBC, CGL)
- calc. (IBC, CGL)
- calc. (IBC, AGL)
- expt. (Ref. 17)
- expt. (Ref. 18)

fit: \( \sim (1 - T/T_c)^{0.5} \)
Figure 3

(a) Graph showing the distribution of $\Psi$ with $z/D$ for different values of $D$ (a.u.).
- Green dashed line for $D = 5.8$
- Black solid line for $D = 29.2$
- Red dotted line for $D = 52.5$

(b) Graph showing the exponential decay and power decay ($\sim D^{-0.17}$) of $B_{c2}$ (Tesla) as a function of $D$ (a.u.).
- Black squares represent the calculation result.
- Blue solid line represents the exponential decay.
- Red dotted line represents the power decay ($\sim D^{-0.17}$).
Figure 4

(a) 

(b) 

$B_{c2}$ (Tesla) vs $M_{\perp}$ (a.u.) 

$B_{c2}$ (Tesla) vs $m_{\parallel}$ (a.u.)
Figure 5

(a) $\alpha_0$ (a.u.)
- 3.8E-3
- 1.9E-3
- 7.8E-5

(b) $B_{c2}$ (Tesla)
- calculation
- linear fit

$\Phi$

D(a.u.)

$\alpha_0$ (a.u.)

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

0 5 10 15 20 25 30

500 550 600 650 700 750 800

-0.0045 -0.0030 -0.0015 0.0000
Figure 6

(a) **Calculations of exponential decay**

(b) **Power decay**

\[ B_{z2} \text{(Tesla)} \sim \frac{1}{D} \]

\[ D = 5.8 \text{ a.u.} \]

\[ D = 52.5 \text{ a.u.} \]
Figure 7

(a) 

(b) 

$\Psi$ 

$z$(a.u.) 

$B_{c2}$(Tesla) 

$\frac{T}{T_c}$ 

- calculation 
- square-root fit