Possible *d*-wave superconductivity in borocarbides: Upper critical field of YNi_2B_2C and $LuNi_2B_2C$

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The upper critical field of a three-dimensional version of *d*-wave superconductors in a variety of field configurations is analyzed theoretically within the weak-coupling model. The present theory describes the main features of upper critical fields observed recently in YNi_2B_2C and $LuNi_2B_2C$. This strongly suggests that the underlying superconductivity in borocarbides should be of *d* wave type. [S0163-1829(98)03534-6]

After a few years of hot controversy it appears that *d*-wave superconductivity in the hole-doped high-T_c cuprates is finally established.[1,2] *d*-wave superconductivity manifests itself as fourfold symmetry of the vortex state when a magnetic field is applied either parallel to the *c* axis or in the *a*-*b* plane.[3] In particular in a magnetic field parallel to the *c* axis the vortex lattice in the vicinity of the upper critical field is shown to be square titled by 45° from the *a* axis except in the immediate vicinity of the transition temperature T_c.[4] This work has recently been extended for a small magnetic field.[5] The square vortex lattice is stable indeed in a wider field region. Such vortex lattices though elongated in the *a* direction have been seen by small-angle neutron scattering[6] (SANS) and scanning tunneling microscopy[7] (STM) both in YBCO monocrystals at low temperatures and small magnetic fields. On the other hand, in a magnetic field within the *a*-*b* plane a $\cos(4\chi)$ dependence of the upper critical field is predicted[8] where χ is the angle $\vec{B}$ makes from the *a* axis. However, due to the fact that a very high field is involved in high-T_c cuprates, the detection of this fourfold term appears to be rather difficult.

Therefore, it was quite a surprise for us that both the square vortex lattices in magnetic fields parallel to the *c* axis and the χ dependence of H_{c2} in a field within the *a*-*b* plane have been seen recently in a number of borocarbides $ErNi_2B_2C$, YNi_2B_2C, and $LuNi_2B_2C$. Indeed both SANS (Refs. 9,10) from borocarbides $ErNi_2B_2C$, YNi_2B_2C, and $LuNi_2B_2C$ and STM from YNi_2B_2C (Ref. 11) demonstrate that the vortex lattice is square titled by 45° from the *a* axis in a magnetic field parallel to the *c* axis and $H>0.375$ T.[11] Further a beautiful $\cos(4\chi)$ term is detected in the upper critical field with a magnetic field within the *a*-*b* plane in $LuNi_2B_2C$.[12] The authors of the above papers tried to interpret these observations in terms of an ordinary *s*-wave superconductor with the Fermi surface with tetragonal distortion. However, we propose to interpret the upper critical field in borocarbides in terms of a three-dimensional (3D) version of $d_{x^2-y^2}$ superconductivity. Unfortunately there is still no conclusive evidence for the *d*-wave superconductivity for borocarbides. However, the appearance of the above superconductivity in the proximity of the antiferromagnetic phase[13,14] or in coexistence with the antiferromagnetic phase clearly indicates Coulomb dominance rather than electron-phonon interaction dominance in borocarbides. Further a recent specific heat data of $LuNi_2B_2C$ in the absence of magnetic field exhibits clearly the power law in *T* rather than exponential behavior.[15] Furthermore, in the vortex state the specific heat clearly indicates the presence of the $\sqrt{B}$ term, which signals the presence of the nodes in $\Delta(\vec{k})$.[16]

In the following we shall show that the upper critical field for a variety of field configurations in a 3D version of *d*-wave superconductivity describes reasonably well experimental data obtained from $LuNi_2B_2C$ (Ref. 12) and YNi_2B_2C.[17] Since the borocarbides are almost isotropic, there will be a possible choice of $\Delta(\vec{k})$ even it is of *d* wave: $\Delta(\vec{k})\propto\cos(2\phi)$ or $\Delta(\vec{k})\propto\sin^2\theta\cos(2\phi)$. A preliminary analysis of $H_c(T)$ and $H_{c2}(T)$ suggests that the first *d*-wave model works much better than the second. Therefore in this paper we limit ourselves to a 3D version of a *d*-wave superconductor. In other words, although the Fermi surface in borocarbides is almost a sphere, we take the same $\Delta(\vec{k})$ as in the hole-doped high-T_c cuprates. We will take this as a strong evidence for *d*-wave superconductivity in borocarbides.[5,18] Of course it is highly desirable to have the node and the phase sensitive experiments in borocarbide superconductors as in high-T_c cuprate superconductors.

Upper critical field in $\vec{B}\|\vec{c}$. Within the weak coupling model for a 3D version of *d*-wave superconductivity the upper critical field for $\vec{B}\|\vec{c}$ is given by[4]

$$-\ln t=\int_0^\infty\frac{du}{\sinh u}\{1-\langle\exp(-\rho u^2\sin^2\theta)\times(1+2C\rho^2u^4\sin^4\theta)\rangle\},\tag{1}$$

$$-C\ln t=\int_0^\infty\frac{du}{\sinh u}\left\{C-\left\langle\exp(-\rho u^2\sin^2\theta)\left[\frac{1}{12}\rho u^2\sin^4\theta+C\left(1-8\rho u^2\sin^2\theta+12\rho^2u^4\sin^4\theta-\frac{16}{3}\rho^3u^6\sin^6\theta+\frac{2}{3}\rho^4u^8\sin^8\theta\right)\right]\right\rangle\right\}\tag{2}$$

where $t=T/T_c$, $\rho=2e^2v^2H_{c2}(T)/(4\pi T)^2$, $\sin^2\theta=1-z^2$, and $\langle\cdots\rangle=\int_0^1dz\ldots$. Here v is the Fermi velocity and we assumed that it is isotropic. In the case of the *z*-axis anisot-

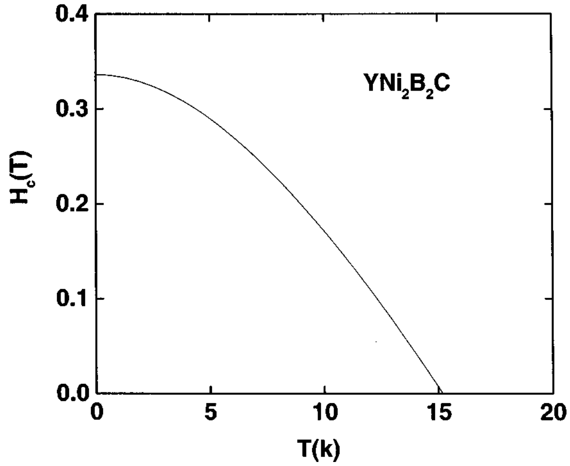

FIG. 1. The thermodynamically critical field of a d-wave superconductor is shown as a function of T. Here we adjust the slope of $H_c(T)$ at $T=T_c$ with the experimental value (Ref. 17).

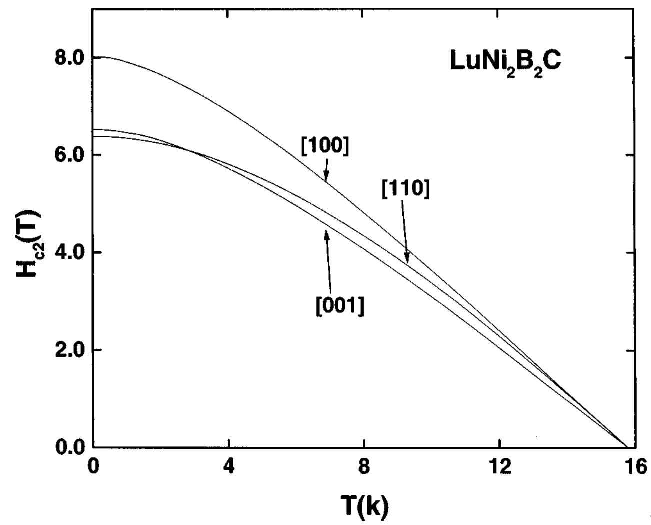

FIG. 3. The same as in Fig. 2 but for $m_c/m_a=1.35$. The temperature dependences are compared with the experimental data for $LuNi_2B_2C$ (Ref. 12).

ropy in the Fermi velocity this effect is readily incorporated. Here we assumed that the order parameter $\Delta(\vec{r},\vec{k})$ is given by

$$\Delta(\vec{r},\vec{k})\propto\cos(2\phi)[1+C(a^{+})^{4}]|0\rangle \tag{3}$$

as in d-wave superconductivity[4] where $|0\rangle$ is the Abrikosov state in s-wave superconductivity, a^{+} is an analog of the raising operator, and ϕ is the angle $\vec{k}$ in the a-b plane makes from the a axis. Hence Eqs. (1) and (2) are analogous to the one in the quasi-two-dimensional system except for an additional coefficient $\sin^2\theta$.

In Fig. 1 we show the thermodynamic critical field taken from Ref. 19, since the thermodynamic properties are the same for the 3D system as well. Compared with the experimental result from YNi_2B_2C,[17] the theory predicts a $H_c(0)$ somewhat larger (about 20%) than the one observed experimentally. For comparison we adjust that the slopes $\partial H_c(T)/\partial T$ at $T=T_c$ with the experimental data. The upper critical field H_{c2} and the coefficient $C(t)$ are obtained numerically and shown in Figs. 2, 3, and 4 as a function of t, respectively. For comparison we include the corresponding one in Fig. 2 for the quasi-2D system.[4] The upper critical field of the 3D system increases somewhat faster than the one for the 2D system with decreasing temperature. On the other hand, the observed $H_{c2}(t)$ of both $LuNi_2B_2C$ and YNi_2B_2C exhibit even faster (about 20%) increases at lower temperature than the present theory. $C(t)$ for the 3D s ystem is almost identical but not equal to the one in the 2D system.

Upper critical field in $\vec{B}$ in the a-b plane. The upper critical field in a magnetic field within the a-b plane is obtained from[8]

$$-\ln t=\int_0^\infty \frac{du}{\sinh u}\{1-\langle[1+\cos(4\chi)\cos(4\phi)] \times\exp(-X)[1+2C\rho u^2(\sin^2\theta\sin^2\phi-\cos^2\theta)]\rangle\}, \tag{4}$$

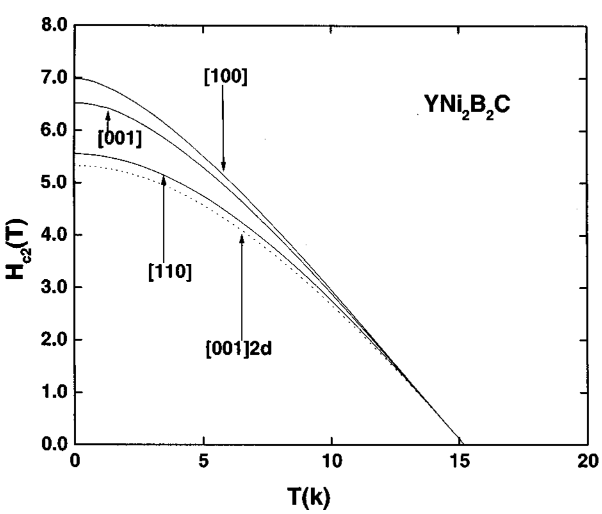

FIG. 2. The upper critical fields for different field direction for $m_c/m_b=1$ are shown as a function of temperature. The temperature dependences are similar to those observed in YNi_2B_2C (Ref. 17).

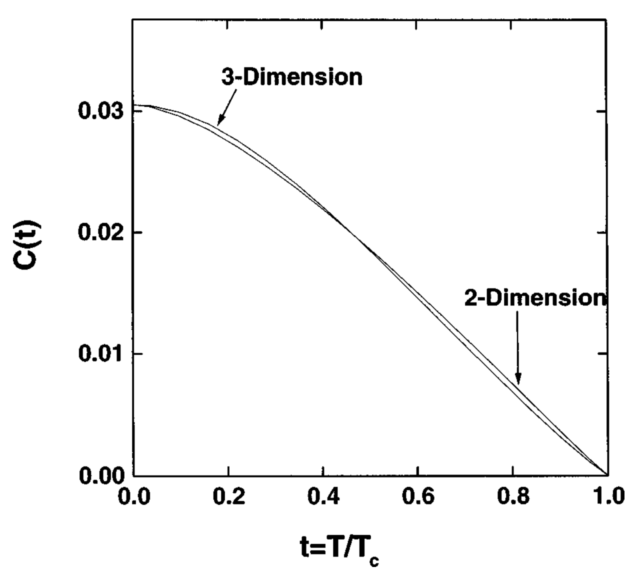

FIG. 4. The coefficient $C(t)$ for the 2D case and our 3D case are shown as a function of $t=T/T_c$. These are very similar but not identical.

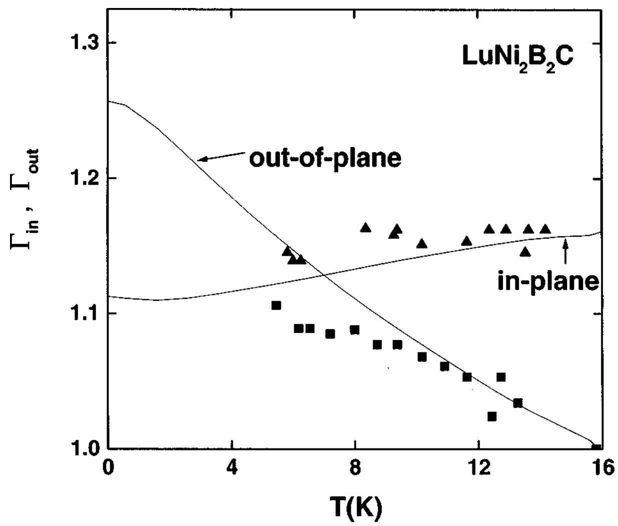

FIG. 5. The out-of-plane and the in-plane anisotropies are shown as a function of temperature. The black squares are the experimental data taken from (Ref. 12).

$$-C\ln t=\int_0^\infty \frac{du}{\sinh u}\{C-\langle[1+\cos(4\chi)\cos(4\phi)]\times\exp(-X)[2\rho u^2(\sin^2\theta\sin^2\phi-\cos^2\theta)+C(1-4X+2X^2)]\rangle\},\quad (5)$$

where $X=\rho u^2(\sin^2\theta\sin^2\phi+\cos^2\theta)$ and we took

$$\Delta(\vec{r},\vec{k})\propto\cos(2\phi)[1+C(a^+)^2]|0\rangle.\quad (6)$$

In Figs. 2 and 3 we show $B\|[100]$ and $[110]$ for $m_c/m_b=1$ and $m_c/m_a=1.35$, respectively. These may be compared with experimental results for YNi_2B_2C and $LuNi_2B_2C$. Indeed these figures describe reasonably well the observed upper critical field. Perhaps the more crucial test of the theory is provided by the in-plane anisotropy $\Gamma_{\rm in}=H_{c2}^{(100)}(T)/H_{c2}^{(110)}(T)$, the average out-of-plane anisotropy $\Gamma_{\rm out}=[H_{c2}^{(100)}(T)+H_{c2}^{(110)}(T)]/2H_{c2}^{(001)}(T)$, and the plane anisotropy $\Gamma=[H_{c2}^{(100)}(T)-H_{c2}^{(110)}(T)]/[H_{c2}^{(100)}(T)+H_{c2}^{(110)}(T)]$. $\Gamma_{\rm in}$ and $\Gamma_{\rm out}$ are shown as a function of T in Fig. 5, while Γ is in Fig. 6 as a function of $1-t$. The black squares and triangles are taken from experiment.[12] Indeed these are in excellent agreement with the theory for $T\geqslant 10$ K (or $t\geqslant 0.625$), since these figures involve no adjustable parameter. However, at lower temperatures the observed $\Gamma_{\rm out}$ is in general smaller than the theory predicts. Another test is provided by the χ dependence of $H_{c2}(t)$ within the a-b plane. We show such a test in Fig. 7. The χ dependence of $H_{c2}(\chi,t)$ is described in a good approximation

$$H_{c2}(t,\chi)=\tfrac{1}{2}[H_{c2}^{(100)}(t)+H_{c2}^{(110)}(t)][1+\Gamma\cos(4\chi)].\quad (7)$$

Again we find an excellent agreement for $T=10$ K, while at lower temperatures the observed anisotropy is somewhat smaller than the theory predicts.

We have analyzed the upper critical field of YNi_2B_2C and $LuNi_2B_2C$ for a variety of field configurations in terms of a 3D version of a $d_{x^2-y^2}$ superconductor in the weak-coupling

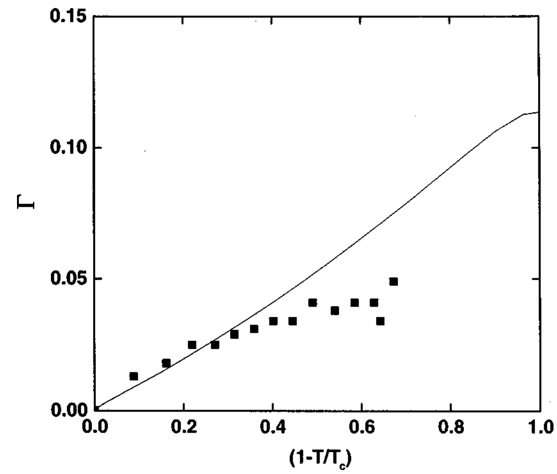

FIG. 6. Γ is shown as a function of 1-t. The data are again from Ref. 12.

limit. We find that the theory describes a variety of features observed experimentally semiquantitatively. In particular both the in plane and out of plane anisotropy in $LuNi_2B_2C$ are described by the present theory satisfactorily for $T\geqslant 10$ K, while some discrepancies set in at lower temperatures. Also $H_{c2}^{(100)}(t)>H_{c2}^{(001)}(t)>H_{c2}^{(110)}(t)$ for YNi_2B_2C and $H_{c2}^{(100)}(t)>H_{c2}^{(110)}(t)>H_{c2}^{(001)}(t)$ for $LuNi_2B_2C$ are correctly given by the present model. Furthermore we expect $H_{c2}^{(110)}(t)<H_{c2}^{(001)}(t)$ at low temperature ($T<3$ K) for $LuNi_2B_2C$. In any case the low-temperature behaviors of the upper critical field will provide a more definite test of the model.

Therefore, though we have to understand the discrepancies below 10 K, we believe these experiments indicate clearly the possible d-wave nature of the underlying superconductivity. Of course further studies on a variety of aspects of borocarbide superconductivity including the phase-sensitive experiment are highly desirable.

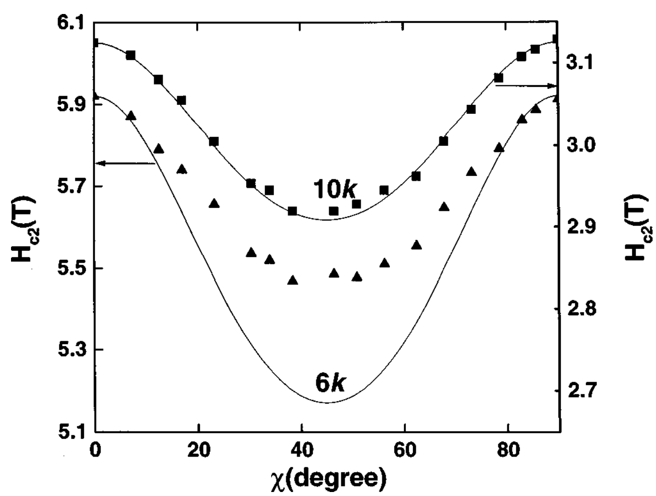

FIG. 7. The χ dependences of the upper critical field of $LuNi_2B_2C$ for $T=10$ and 6 K are compared with the theoretical result (Ref. 12).

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