

Fermi-surface-sheet dependent electron-phonon coupling in a borocarbide superconductor $\text{YNi}_2\text{B}_2\text{C}$

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We performed de Haas-van Alphen (dHvA) oscillation measurements and band-structure calculations for $\text{YNi}_2\text{B}_2\text{C}$. Our improved band structure successfully explained the origins of the large dHvA frequencies β and ζ , which were inexplicable in previous works. By comparing experimental effective masses with band masses, we determined the electron-phonon coupling for each orbit. The results showed a clear Fermi-surface-sheet dependence of the electron-phonon coupling strength, especially highlighting that the coupling for the band-28 sheet is very weak, almost absent for the orbit with $B \parallel c$. This finding is consistent with previous observations of dHvA oscillations from this orbit in the mixed state down to very low fields. Amidst growing interest in high-temperature superconductivity driven by electron-phonon coupling in hydrides under high pressure, this study provides foundational data pivotal to precisely understanding electron-phonon coupling.

de Haas-van Alphen (dHvA) oscillation measurements combined with band-structure calculations are a powerful tool to investigate bulk electronic structures in metals. One can determine not only the shape of the Fermi surface but also the effective mass. The effective mass m^* determined by dHvA measurements is enhanced over the band mass m_{band} by electron-phonon and electron-electron interactions: $m^* = (1 + \lambda)m_{\text{band}}$. Thus one can characterize the many-body interactions in metals by determining the enhancement parameter λ for different cyclotron orbits on different Fermi-surface sheets. Pioneering work was conducted nearly 40 years ago on the electron-phonon coupling superconductor Nb, revealing that the strength of electron-phonon coupling varies across different sheets of the Fermi surface with up to $\pm 40\%$ variation [1]. More recently, it has been reported that the magnitude of electron-phonon coupling in MgB_2 differs significantly between the σ and π bands [2, 3].

dHvA oscillations can also be observed in the mixed state of superconductors: e.g., NbSe_2 [4, 5], A15 superconductors [6–8], borocarbide superconductors [9–12], organic superconductors [13, 14], heavy-fermion superconductors [15–19], MgB_2 [2, 20, 21], KOs_2O_6 [22], and high- T_c cuprates [23, 24]. dHvA oscillations in the mixed state suffer extra damping compared to the normal state. This damping is due to the opening of the superconducting gap, and therefore, by analyzing this damping, it is expected that one can estimate the magnitude of the superconducting gap for each orbit, although, at present, many different theoretical models have been proposed [25–38], and it is unclear which model is the most quantitatively reliable (see, for example, discussion in [36, 39, 40]).

In this paper, we focus on $\text{YNi}_2\text{B}_2\text{C}$, a nonmagnetic member of the rare-earth nickel-borocarbide superconductors [41, 42], with a relatively high superconduct-

ing transition temperature of $T_c = 15.6$ K. Although those borocarbides contain a typical magnetic element Ni, phonon-mediated superconductivity was theoretically suggested [43] and finally confirmed experimentally by the observation of clear isotope effects [44]. Thus the mass enhancement in $\text{YNi}_2\text{B}_2\text{C}$ is basically ascribed to the electron-phonon coupling. Intriguingly, despite the phonon-mediated superconductivity, strong anisotropy in the superconducting gap has been suggested from upper critical field, specific heat, thermal conductivity, and angle-resolved photoelectron spectroscopy measurements [45–48].

Several research groups have conducted dHvA measurements on $\text{YNi}_2\text{B}_2\text{C}$ and a sister compound $\text{LuNi}_2\text{B}_2\text{C}$ to determine the Fermi surface [9, 10, 12, 49–52]. Although comparison to band-structure calculations was partially successful, there was a notable discrepancy: the calculations were unable to explain the origin of the second largest frequency β with $F \sim 7$ kT for $B \parallel c$ (Fig. 1) [12, 52–54]. In addition, a large frequency ζ remained unexplained as well (Fig. 1). Because the β orbit occupies more than 20% of the cross-sectional area of the Brillouin zone, these failures are serious. Intriguingly, the α oscillation arising from a small closed Fermi sheet in $\text{YNi}_2\text{B}_2\text{C}$ could be observed deep in the mixed state, in some cases down to a field as low as $\sim 20\%$ of the upper critical field ($0.2B_{c2}$) [9, 10, 12, 51, 55–57]. It was argued that the gap opening on this sheet is much smaller than gaps on other sheets [51, 57].

In this study, we perform dHvA measurements on $\text{YNi}_2\text{B}_2\text{C}$ for various field directions. We show that our improved band-structure calculation successfully explains the origins of the previously inexplicable β and ζ frequencies. We then compare the experimental effective masses with band masses to determine the mass enhance-

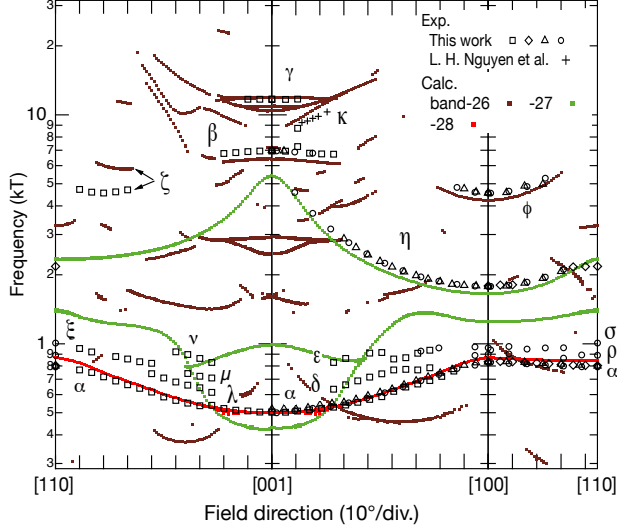


FIG. 1. Experimental vs theoretical dHvA frequencies in $\text{YNi}_2\text{B}_2\text{C}$. Squares, diamonds, triangles, and circles indicate dHvA frequencies experimentally observed in the present four samples of $\text{YNi}_2\text{B}_2\text{C}$. Crosses are from [50]. Dots indicate frequencies calculated from the present band-structure calculation.

ment parameter λ for each orbit. The results clearly show the Fermi-surface-sheet dependence of the mass enhancement. Especially, the mass enhancement for the α orbit is very small, nearly absent for $B \parallel c$. This strongly suggests that the α sheet is passive for superconductivity and hence that the gap on this sheet is small, in line with the observation of dHvA oscillations from the α sheet at very low fields in the mixed state. Although the mass enhancement in $\text{LuNi}_2\text{B}_2\text{C}$ was previously determined in a similar manner [52], the band-structure used in the study was unable to explain the β frequency and also the ϕ frequency (Fig. 1), which restricts the reliability of the obtained results. The recent discovery of high-temperature superconductivity in hydrides under high pressure has sparked renewed interest in the electron-phonon interaction [58, 59]. The precise determination of the Fermi-sheet dependent electron-phonon coupling demonstrated in this study makes an important contribution to such a research trend.

$\text{YNi}_2\text{B}_2\text{C}$ single crystals were grown by a floating zone method [60, 61]. Field-modulation dHvA measurements were performed in a dilution refrigerator installed in a 16-T or a 20-T superconducting magnet [61]. The magnetic field was rotated in the $(1\bar{1}0)$, (010) , and (001) planes. The field angles $\theta_{(1\bar{1}0) \text{ or } (010)}$ and φ are measured from the $[001]$ and $[100]$ axes, respectively. Four samples were measured and gave consistent results.

Figure 2 shows examples of the observed dHvA oscillations and corresponding Fourier transforms. Figure

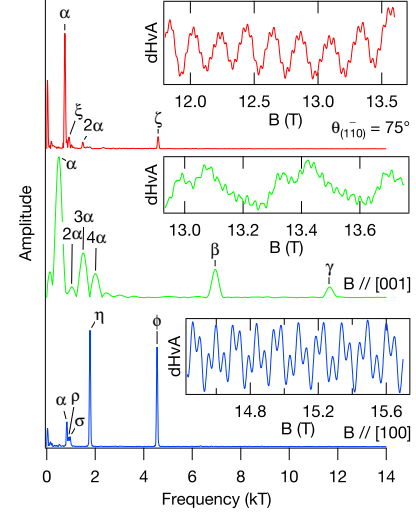


FIG. 2. de Haas-van Alphen oscillation in $\text{YNi}_2\text{B}_2\text{C}$. dHvA oscillations detected by field-modulation technique (inset) and corresponding Fourier transforms are shown for indicated magnetic field directions. The measurement temperatures were 30–50 mK.

1 plots the observed dHvA frequencies as a function of the field direction. According to the Onsager relation, the frequency of the dHvA oscillations is proportional to the k -space area of the observed cyclotron orbit [62]. In the present case, for $B \parallel c$, the frequency $F = 300$ T corresponds to an orbit whose area is about 1% of the cross-sectional area of the Brillouin zone. Many frequency branches were observed as labelled by Greek letters. The frequencies observed in the four samples agree well when the measurement directions overlap. The observed field-angle dependence of the frequencies is in line with previously reported ones [9, 50]. It is also very similar to that reported for $\text{LuNi}_2\text{B}_2\text{C}$ [12, 52].

In order to interpret the observed frequency branches, we calculated the electronic band structure within the local density approximation (LDA), using a full-potential linearized augmented plane-wave (FLAPW) method [61]. Following [54], we shifted the Y d and Ni d levels upward from the LDA levels by 0.11 and 0.05 Ry, respectively. Empirically, such a shift is known to improve the agreement between the calculated Fermi surface and experimental observations [63–67]. This indicates that the relative energy levels of electrons obtained by LDA should sometimes be corrected. We used the experimental lattice parameters: $a = 3.526$ Å, $c = 10.543$ Å, and $z(\text{B}) = 0.358$ [68]. The present calculation is basically the same as that in [54], but a much finer k -mesh ($24 \times 24 \times 8$; 767 k -points in the irreducible Brillouin zone) was used to capture fine details of the Fermi surface.

Three bands cross the Fermi level [Fig. S3(a)], and the calculated density of states is 58.3 states/Ry. This corresponds to the electronic specific heat coefficient of

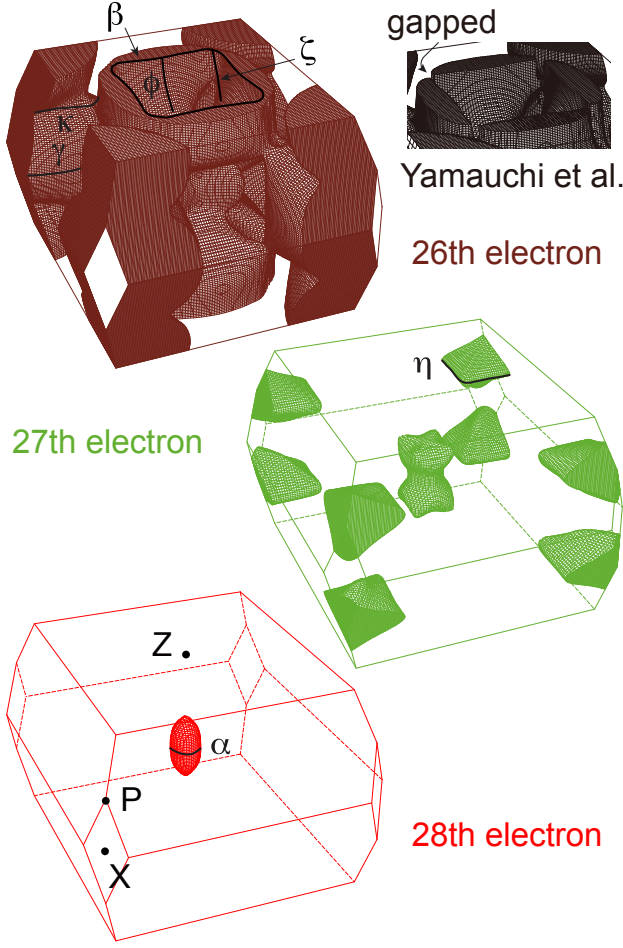


FIG. 3. Calculated Fermi surface in $\text{YNi}_2\text{B}_2\text{C}$. Extremal orbits are indicated. Top right inset shows part of the band-26 electron surface calculated in [54], for comparison.

$\gamma_{\text{band}} = 10.1 \text{ mJ/mol K}^2$, and, compared to an experimental value of $\gamma_{\text{exp}} = 18.2 \text{ mJ/mol K}^2$ [69], gives a Fermi-surface averaged electron-phonon coupling of $\langle \lambda \rangle = \gamma_{\text{exp}}/\gamma_{\text{band}} - 1 = 0.8$. Figure 3 shows the calculated Fermi surface. The 26th band produces the multiply-connected electron sheet at Γ and closed ones at P, and the 28th a closed electron sheet at Γ .

We computed dHvA frequencies based on the calculated band structure (Fig. 1). In the calculation, we shifted the 28th band downward by 5 mRy (68 meV) to achieve a better agreement with the α frequency. Such a small adjustment of the band energy ($\sim 100 \text{ meV}$) is a common practice when comparing theoretical and experimental dHvA frequencies [70–74]. This necessity may arise from numerical errors in the calculations or from electronic correlations that are not sufficiently taken into account within LDA. As seen from Fig. 1, our Fermi surface can explain most of the experimental frequency branches, i.e., α , β , γ , ζ , η , κ , and ϕ , whose correspond-

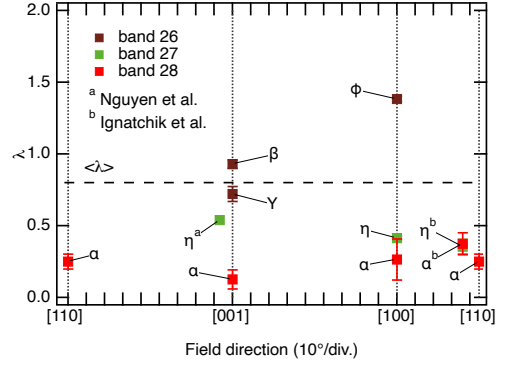


FIG. 4. Mass enhancement parameter $\lambda = m^*/m_{\text{band}} - 1$ in $\text{YNi}_2\text{B}_2\text{C}$. The marks labelled with a and b are based on the effective masses reported in [50, 77]. The horizontal dashed line indicates the Fermi-surface averaged mass enhancement $\langle \lambda \rangle$.

ing orbits are depicted in Fig. 3 [for ζ and ϕ , see also Fig. S3(c)]. For the ζ branch, there is a slight difference between the experimental and calculated frequencies. However, this frequency difference corresponds to only a small energy shift of about 9.6 mRy (130 meV) within an effective-mass approximation. (We did not shift the 26th band because it would affect multiple frequency branches.) The remaining branches may be assigned to the band-27 Γ -centered pocket. However, since this pocket is small (with a cross-sectional area on the order of 1% of the Brillouin zone) and has a relatively complex shape, the numerical agreement of the frequencies is not satisfactory.

It is noteworthy that the present calculation can explain branches β and ζ , which could not be explained by previous band-structure calculations [54, 75, 76]. The band-26 sheet surrounding the ΓZ line looks like a flower with four petals. In the present calculation, the four petals are connected on the Z plane ($k_z = 2\pi/c$), which allows orbits β and ζ [Fig. 3, see also Figs. S3(b) and (c)]. In the previous calculation of [54] (top right inset of Fig. 3), the four petals are not connected on the Z plane, and there are gaps between adjacent petals.

We determined effective masses for frequencies observed for $B \parallel [110]$, $[001]$, and $[100]$ by measuring temperature dependence of the oscillation amplitudes [61]. We then determined the mass enhancement parameters $\lambda = m^*/m_{\text{band}} - 1$ by comparing the experimental effective masses and theoretical band masses (see Table SI). We plotted the obtained mass enhancement parameters in Fig. 4, where we also plotted values estimated from the effective masses reported in [50, 77] together (labelled with a and b). λ varies by about an order of magnitude, from 0.13(7) for the α orbit with $B \parallel c$ to 1.38(2) for the ϕ orbit with $B \parallel a$. This indicates a significantly larger variation in comparison with MgB_2 , where λ differs at

most by a factor of three: ~ 0.4 for the π band and ~ 1.1 for the σ band [3].

Figure 4 clearly shows the Fermi-surface-sheet dependence of the mass enhancement. The mass enhancement decreases in the order of the band-26 sheet, band-27 P-centered sheet, and band-28 sheet. The improved band-structure calculation in the present study enabled us to observe this trend clearly. The λ values for the band-27 P-sheet and the band-28 sheet are significantly smaller than the Fermi-surface average $\langle \lambda \rangle$ (horizontal dashed line) determined from specific heat measurements, suggesting that these parts of the Fermi surface may account for the multiband superconductivity observed in this compound through various experiments [45–47]. Band-27 constitutes approximately 20% of the total density of states (DOS) at the Fermi level, although the contribution of band-28 is minor. However, it is difficult to confirm the pointlike minimum of the gap reported by ARPES [48].

Previous results on $\text{LuNi}_2\text{B}_2\text{C}$ did not show such a clear trend [52]: The mass enhancements of the cushion and sphere sheets in [52], which correspond to our band-27 P-sheet and band-28 sheet, respectively, showed a crossover depending on the magnetic field direction. The mass enhancement for the branched FS in [52], which corresponds to our band-26 sheet, was no larger than that for the cushion sheet (corresponding to our band-27 P-sheet). In addition, the mass enhancement for the cube sheet in [52], which corresponds to our band-27 Γ -centered sheet, was reported to largely vary with the field direction: it was ~ 1 for [100] but became ~ 2.7 for [001] [52]. The lack of a clear trend in the mass enhancement in [52] might reflect the inadequate agreement between their calculated Fermi surface and the experimental dHvA results. Specifically, their Fermi surface fails to explain the β and ζ frequencies, and its calculated frequencies for the α orbit show poor agreement with the experimental data [52].

Figure 4 shows that the mass enhancement for the band-28 electron sheet is very weak. Especially, it is only 0.1(1) for the field direction of [001]. This is very consistent with the conclusion drawn from the observation of dHvA oscillations from this sheet far below B_{c2} for $B \parallel c$ that the gap on this sheet is much smaller than gaps on other sheets [51, 57]. It is noteworthy that the two independent methodologies based on dHvA measurements, i.e. estimation of the mass enhancement (present study) and observation of dHvA oscillations in the mixed state [51, 57], reached the same conclusion that the band-28 sheet is passive with respect to superconductivity in $\text{YNi}_2\text{B}_2\text{C}$.

The mass enhancement due to the electron-phonon coupling in $\text{YNi}_2\text{B}_2\text{C}$ was theoretically studied in [78]. The largest electron-phonon coupling was found on the band-27 Γ -centered sheet. Unfortunately, we were unable to identify dHvA frequencies arising from this sheet

with certainty in the present study. The study [78] indicated that the second most strongly coupled sheet was the band-26 sheet, while the third the band-27 P-sheet. This is consistent with the present result (Fig. 4). For the band-28 sheet, the band-structure calculation in [78] wrongly predicted two closed pockets around Γ , and hence comparison cannot be made with the present result.

In summary, we performed dHvA measurements on $\text{YNi}_2\text{B}_2\text{C}$. Our improved band structure calculation successfully explained most of observed frequency branches. Especially, it revealed the origins of the previously inexplicable large frequencies β and ζ . We determined the many-body mass enhancement parameter λ by comparing experimental effective masses with band masses. The results showed a clear Fermi-sheet dependence of the electron-phonon coupling that the coupling weakens in the order of the band-26 sheet, band-27 P-sheet, and band-28 sheet. The electron-phonon coupling for the band-28 sheet is very weak, almost absent for $B \parallel c$. This strongly suggests that the superconducting gap on this sheet is small and hence is in line with the previous reports that dHvA oscillations from this sheet can be observed deep in the mixed [51, 57]. There was a certain level of agreement between the electron-phonon coupling experimentally deduced in this study and that theoretically calculated in [78]. Considering recent discoveries of electron-phonon coupling high-transition-temperature superconductivity in hydrides [58, 59], accurate theoretical calculations of electron-phonon coupling are of significance. This study provides essential input for the development of such methods. In addition, our results clearly demonstrate that strong electron-phonon coupling can be realized in compounds containing light elements such as carbon or boron, even when heavier elements like Ni and Y are present. This provides an important guideline for the future exploration of superconducting materials.

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