

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

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(Dated: June 23, 2026)

CRYSTAL GROWTH AND CHARACTERIZATION

Single crystals of $\text{YNi}_2\text{B}_2\text{C}$ were grown by a floating zone method without a crucible to avoid impurity inclusions into grown crystals, as detailed in [SM1]. The crystals were examined by SEM, EPMA and X-ray diffraction technique and found to be of high quality without any secondary phase. Details of the results of these characterizations can be found in Refs. [SM1–SM3] (the dHvA measurements reported in the present paper were performed between 1995 and 1997, in parallel with these characterizations). The lattice parameters were $a = 3.5265(1)$ and $c = 10.5415(3)$ Å, which are in excellent agreement with those reported in [SM4]. The superconducting transition was observed at $T_c = 15.6$ K (onset) with a very narrow transition width of 0.7 K [SM1]. The residual resistivity ratio RRR was 29.3 with electrical current applied along the a -axis, and the resistivity at T_c was $2.89 \mu\Omega\text{cm}$.

DE HAAS–VAN ALPHEN MEASUREMENTS

The reported dHvA measurements were performed with the field-modulation technique [SM5, SM6], and detection was made at the second harmonic of the modulation frequency. The modulation frequency and amplitude were typically 67 Hz and 10 mT, respectively. The insets of Fig. 2 (main text) show examples of raw data without background subtraction. The effective mass m^* for each frequency (orbit) was determined by fitting the temperature reduction factor R_T of the Lifshitz-Kosevich formula to the experimental temperature dependence of the oscillation amplitude, which was determined by Fourier transformation: $R_T = X/\sinh X$, where $X = rK\mu^*T/B$ for a fundamental ($r = 1$) or a r -th harmonic frequency, $\mu^* = m^*/m_e$, and the coefficient K is 14.69 T/K [SM5]. Figures S1 and S2 show examples of mass determination.

BAND-STRUCTURE CALCULATIONS

The band-structure calculations are carried out by using FLAPW method based on the local density approximation (LDA) formula proposed by Gunnarsson and Lundqvist [SM7]. As mentioned in the main text, we shifted the Y d and Ni d levels upward from the LDA levels by 0.11 and 0.05 Ry, respectively. The method of the calculation and the parameters used are the same as those in the previous one [SM8], except the number of sampling k -points. The experimentally observed lattice constants are used: $a = 3.526$ Å, $c = 10.543$ Å, and $z(\text{B}) = 0.358$ [SM4]. Muffin-tin (MT) radii are set as $0.1747a$, $0.1358a$, $0.1010a$, and $0.1010a$ for Y, Ni, B, and C respectively. Core electrons (Kr-core minus $4p^6$ for Y, Ar-core minus $3p^6$ for Ni, He core for B and C) are calculated inside the MT spheres. $4p^6$ electrons on Y and $3p^6$ electrons on Ni are calculated as valence electrons by using the second energy window. The scalar relativistic effects are taken into account for all electrons, and the spin-orbit coupling is considered self-consistently for all valence electrons inside the MT spheres as in a second variational procedure. The LAPW basis functions are truncated at $|\mathbf{k} + \mathbf{G}_i| = 4.01 \times 2\pi/a$ corresponding to 403 LAPW functions at the Γ point.

The sampling 767 k -points (divided by 24, 24, and 8) are uniformly distributed in the irreducible 1/16th of the bct Brillouin zone (BZ), instead of 369 k -points (divided by 16, 16, and 8) in the previous work [SM8]. Accordingly, the energies are calculated at about twice as many points within each $k_z = \text{constant}$ plane compared to the previous study. To draw the perspective view of the Fermi surfaces and calculate the extremal areas, the energy eigenvalues are interpolated at the 226,981 mesh points.

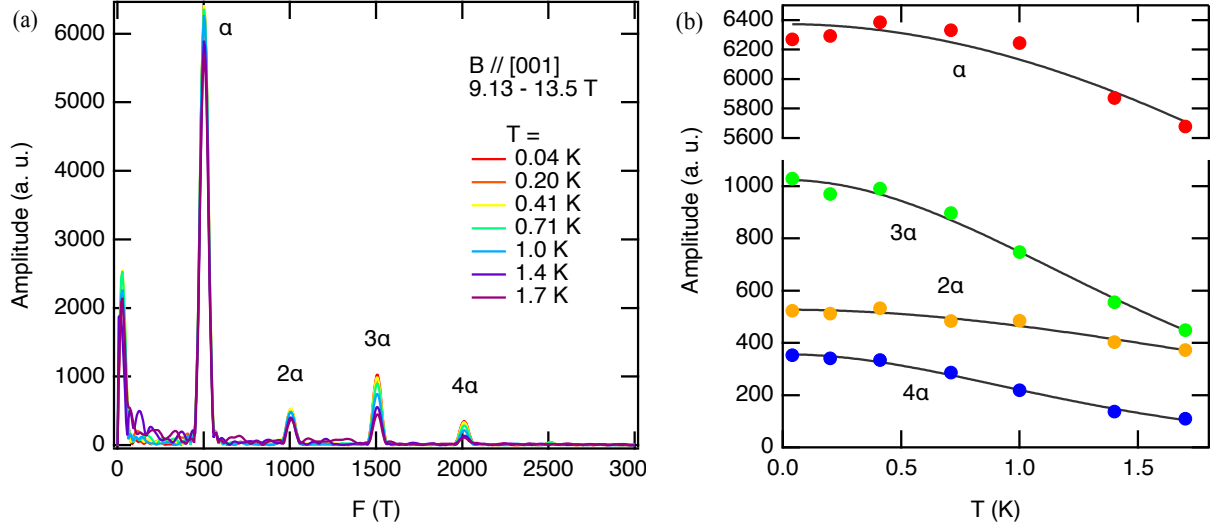


FIG. S 1. Effective mass of α . (a) Fourier transforms of oscillations measured with $B \parallel c$ at indicated temperatures. (b) Temperature dependences of oscillation amplitudes for α , 2α , 3α , and 4α . The solid lines are fits to R_T , which yield $m^*/m_e = 0.36(3)$, $0.33(2)$, $0.35(1)$, and $0.33(1)$, respectively, where the errors in parentheses are numerical fitting errors. From the weighted average, we conclude $m^*/m_e = 0.34(2)$.

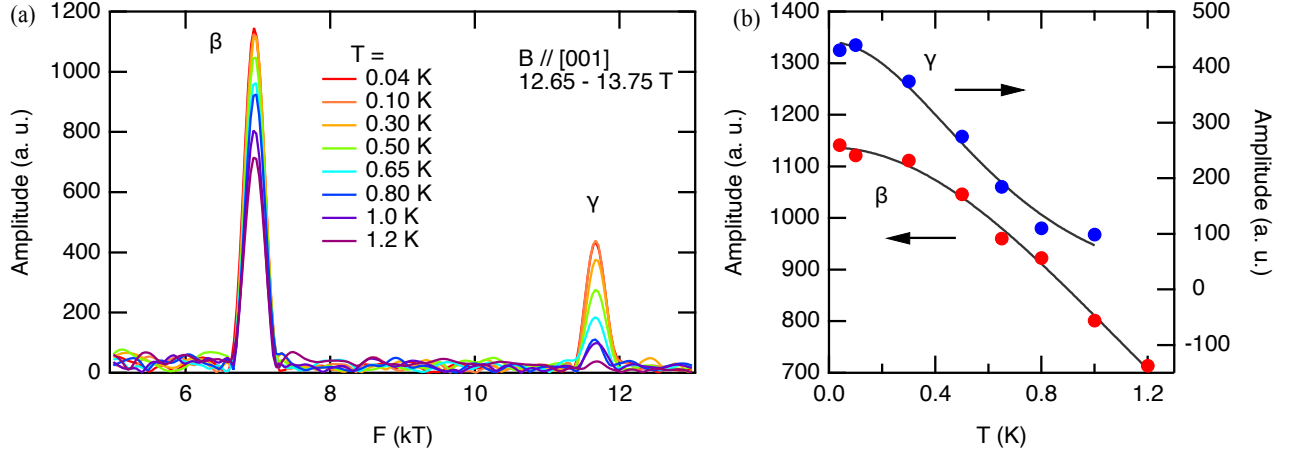


FIG. S 2. Effective masses of β and γ . (a) Fourier transforms of oscillations measured with $B \parallel c$ at indicated temperatures. (b) Temperature dependences of oscillation amplitudes for β and γ . The solid lines are fits to R_T , which yield $m^*/m_e = 1.32(3)$ and $3.3(1)$, respectively, where the errors in parentheses are numerical fitting errors.

ESTIMATION OF λ

Table S1 provides the source data for the mass enhancement factor λ shown in Fig. 4.

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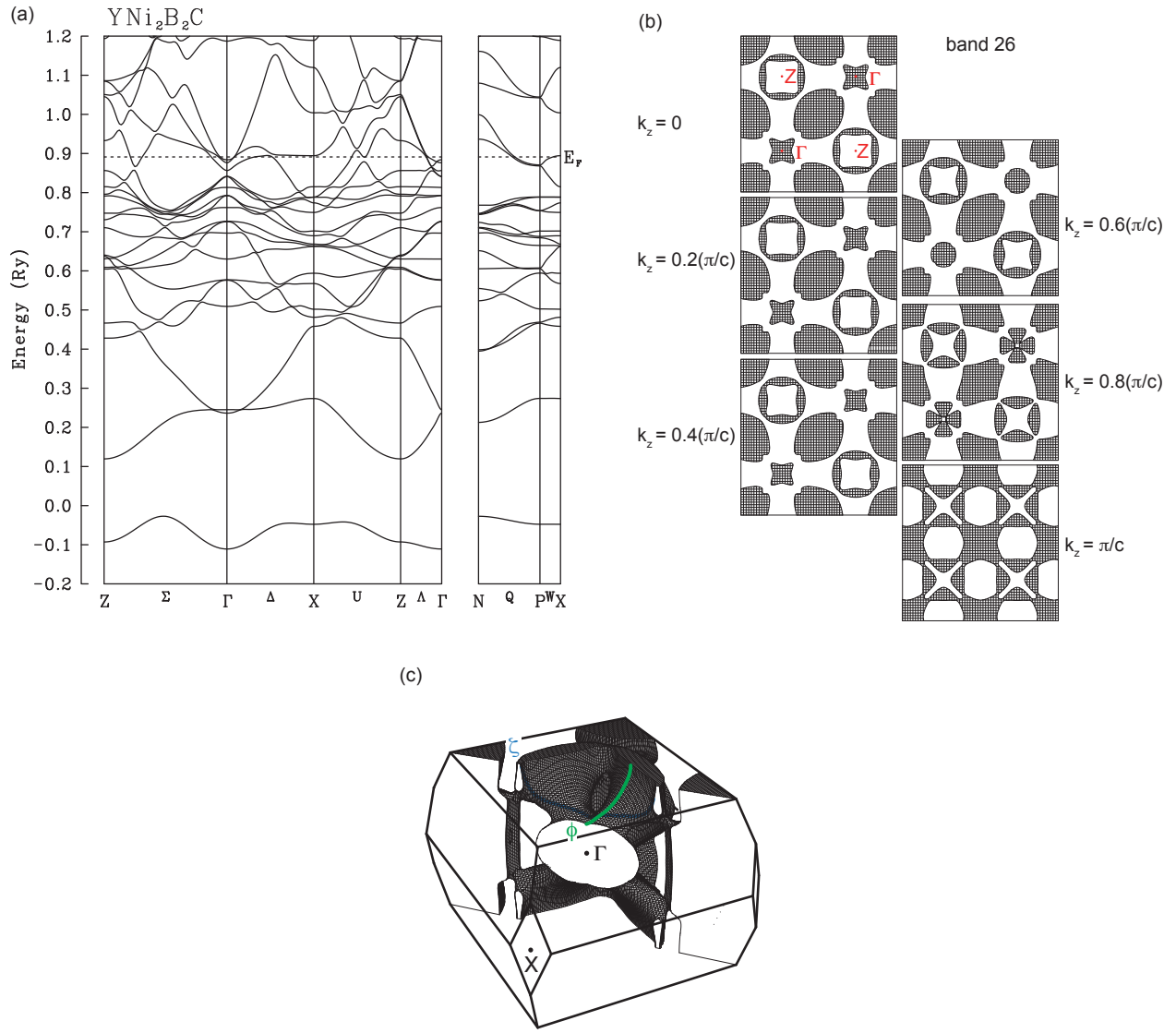


FIG. S 3. (a) Calculated band structure. (b) Cross-sections of the band-26 Fermi surface. (c) ζ and ϕ orbits on the band-26 Fermi surface.

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TABLE S I. Experimental and calculated dHvA frequencies and masses, and mass enhancements calculated as $\lambda = m^*/m_{band}-1$. The errors quoted for the effective masses are numerical fitting errors, from which the errors for λ were derived.

θ ($^\circ$)	Branch	Experiment		Calculation		λ
		F (kT)	m^*/m_e	F (kT)	m_{band}/m_e	
[110]	α	0.79	0.48(2)	0.84	0.38	0.25(5)
[001]	γ	11.7	3.3(1)	11.9	1.9	0.72(5)
[001]	β	7.0	1.32(2)	6.4	0.68	0.93(3)
[001]	α	0.50	0.34(2)	0.50	0.30	0.13(7)
[100]	ϕ	4.5	1.27(1)	4.2	0.53	1.38(2)
[100]	η	1.8	1.86(2)	1.7	1.32	0.41(2)
[100]	α	0.83	0.53(6)	0.87	0.42	0.3(1)
$\theta_{(1\bar{1}0)} = 7^\circ$ ^a	η	5.5	3.2	4.8	2.1	0.54
$\varphi = 36^\circ$ ^b	η		2.7(1)	2.1	2.0	0.35(5)
$\varphi = 36^\circ$ ^b	α		0.54(3)	0.84	0.39	0.37(8)

^a From [SM9]. The field direction is 7° from [001] towards [110]. The frequency was read from Fig. 2 of [SM9].

^b From [SM10]. The field direction is 36° from [100] towards [110]. The frequency values were not given in [SM10].