Fermi surfaces of YFe_2 and YNi_2

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Abstract

Electronic structures and Fermi surfaces of YFe_2 and YNi_2 with a cubic Laves phase structure are calculated in the non-magnetic state by using an FLAPW method. Angular dependences of the extremal cross-sectional areas of the Fermi surfaces of these compounds are also calculated.

Key words: YNi_2, YFe_2, Fermi surface, dHvA frequency

Recently, magnetic properties of intermetallic compounds of rare-earth (R) and 3d transition elements, RM_2 (M=Mn, Fe, Co and Ni), have been studied intensively. Among them, yttrium compounds YM_2 with the cubic Laves phase ($MgCu_2$-type) structure are widely known as possessing interesting magnetic properties associated with 3d electrons in M atoms [1]. Many theoretical and experimental studies on the magnetic properties have already been carried out for antiferromagnetic YMn_2, ferromagnetic YFe_2, paramagnetic YCo_2 and YNi_2. However, direct studies on the Fermi surface itself, e.q., dHvA frequency, have not been done so far, except for theoretical calculations for YCo_2 [2]. In this paper, the angular dependences of the extremal cross-sectional area (ECSA) of the Fermi surfaces of the non-magnetic YFe_2 and YNi_2 are calculated. The calculations for non-magnetic YMn_2 are published elsewhere [3].

The band structure calculations for the non-magnetic YFe_2 and YNi_2 are carried out by using a self-consistent FLAPW method. The local density approximation in the Gunnarsson and Lundqvist formula [4] is adopted to construct the exchange-correlation terms for the oneelectron potential. The spin-orbit interaction is not included. Observed lattice constants are used in the present calculations.

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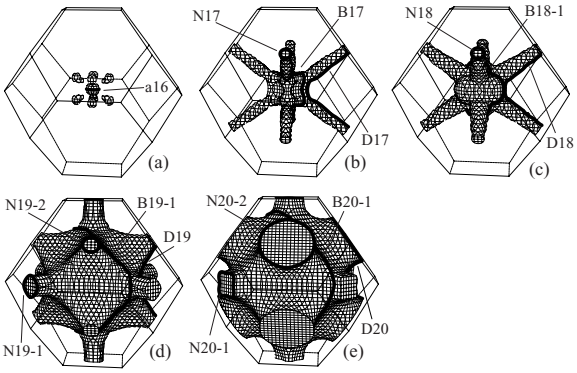

Fig. 1. Hole surfaces of non-magnetic YFe_2. (a)∼(e) are those of 16th∼20th bands, respectively.

For constructing basis function, we used the criteria $l_{\max} = 7$ inside the muffin-tin (MT) spheres and $|k+G_i| \leq K_{\max} = 8.5\times(2\pi/a)$ outside the MT spheres, where k is a wave vector in the first Brillouin zone, G_i the reciprocal lattice vector. The final potential is constructed self-consistently from eigenstates at 85 sampling $k-$points in the irreducible 1/48 Brillouin zone (IBZ). To obtain a final band structure, we selected 231 sampling $k-$points in the IBZ. The MT radii of Y and M(=Fe,Ni) are taken as 0.165 and 0.155 in a unit of lattice constant a. The convergence is achieved as that the difference between input and output potentials becomes smaller than 10^{-7} Ryd.

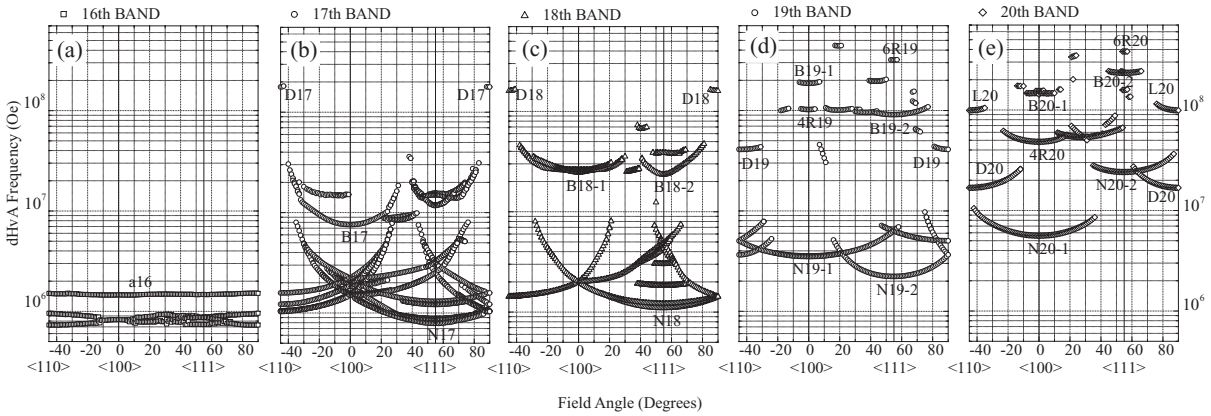

Fig. 3. Angular dependence of the calculated extremal cross-sectional areas, corresponding to experimental dHvA frequencies, of the Fermi surfaces in YFe_2. (a)∼(e) are dHvA frequencies of 16th∼20th bands, respectively.

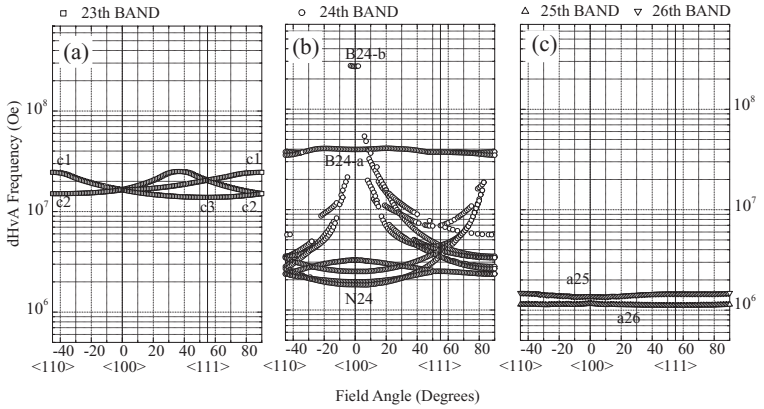

Fig. 4. Angular dependence of the calculated extremal cross-sectional areas, corresponding to experimental dHvA frequencies, of the Fermi surfaces in YNi_2. (a),(b) and (c) are dHvA frequencies of 24th,25th and 26th bands.

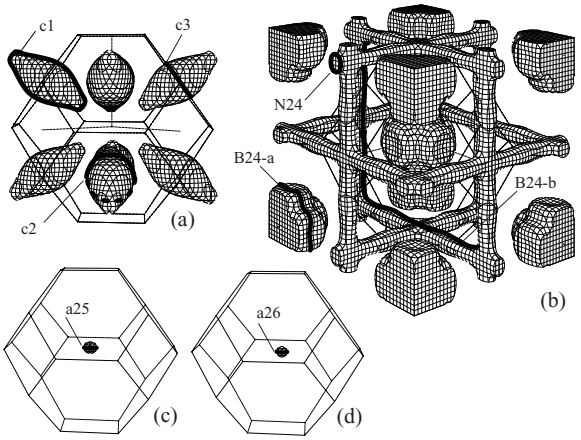

Fig. 2. Fermi surfaces of non-magnetic YNi_2 (a):hole surface of 23th band. (b):electron surface of 24th band. (c):electron surface of 25th band. (d):electron surface of 26th band.

The electronic specific heat coefficient γ is estimated from the calculated density of states. The calculated values of γ are 25.0 and 3.67 mJ/mol·K^2 for the non-magnetic YFe_2 and YNi_2. The observed γ for YNi_2 [5] is close to our calculated one.

The calculated results of the Fermi surfaces and ECSA for the non-magnetic YFe_2 and YNi_2 are shown in Figs. 1∼4. The symbols shown on the curves of ECSA in Figs. 3 and 4 correspond to those for the Fermi surfaces in Figs. 1 and 2, respectively. Measurements of the dHvA frequency are desired to confirm the present calculations.

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