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De Haas-van Alphen effect in LaAl_2

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Résumé. — La surface de Fermi de la phase cubique de LaAl_2 est étudiée à l'aide de l'effet de Haas-van Alphen (dHvA). Trois groupes de fréquences dHvA sont observés entre $F = 0,15$ et $82,7$ MG avec des masses cyclotron entre $m^*/m_0 = 0,11$ et $1,70$. Les fréquences dHvA les plus élevées correspondent à une grande surface Fermi en substance sphérique mais avec des bosses en direction de $\langle 100 \rangle$ et sont en accord avec les calculs de bandes APW [1]. Des calculs de bandes plus détaillés, self-consistent et relativistiques sont nécessaires pour interpréter les fréquences plus basses comme étant dues à de petites surfaces (trous) et pour décider de l'influence des bandes f de La près de E_F sur les propriétés électroniques de LaAl_2 .

Abstract. — The Fermi surface of the cubic Laves phase LaAl_2 is studied by means of de Haas-van Alphen (dHvA) effect measurements. Three groups of dHvA frequencies are observed between $F = 0.15$ and 82.7 MG with cyclotron masses between $m^*/m_0 = 0.11$ and 1.70 . The highest dHvA frequencies correspond to a large Fermi surface essentially spherical but with bumps in $\langle 100 \rangle$ directions and are in agreement with APW energy band calculations [1]. More detailed self-consistent relativistic energy band calculations are necessary in order to interpret the lower dHvA frequencies as due to small (hole) surfaces and then to decide how the nearby f-bands of La affect the electronic properties of LaAl_2 .

1. Introduction. — The cubic Laves phases compound LaAl_2 is very attractive as it serves as an exemplary host for studying especially the magnetic properties of 4f rare earth impurities [2]. This short note deals with electronic properties of the matrix. In the APW energy band calculations for LaAl_2 [1] an analysis of the occupied band states in terms of angular momenta shows a 30 % f-state admixture to the total density of states at the Fermi energy E_F . The de Haas-van Alphen (dHvA) effect, being sensitive to electrons at E_F provides an adequate test of those calculations.

2. Experimental techniques and results.— Single crystals of LaAl_2 typically with 1.2 mm in diameter, about 5 mm long and with residual resistivity ratios around 150 after annealing were cut by spark erosion from large single crystals grown by the Czochralski technique using high purity La (99.996 %) and Al (99.999 %). Details of the setup for the present dHvA experiment are given elsewhere [3]. The frequency spectrum at each sample orientation was determined by means of fast Fourier transform techniques. The present status of the angular variation of the dHvA frequencies in the (100) and (110) planes are shown

on a logarithmic scale in figure 1. Three groups of frequencies cover a range of more than two orders of magnitude. The group of ε oscillations is degenerate

Fig. 1. — Angular dependence of de Haas-van Alphen periods found in LaAl_2 .

in $\langle 111 \rangle$ directions. In table I we list some measured frequencies and effective cyclotron masses for the three symmetry directions $\langle 100 \rangle$, $\langle 111 \rangle$, and $\langle 110 \rangle$ together with some estimated areas from the energy band calculations [1] and unpublished independent experimental data [4].

Table I. — *Extremal areas and effective cyclotron masses for LaAl_2 .*

Oscillation Orientation	10 ⁶ G this exp.	10 ⁶ G exp. [4]	10 ⁶ G APW [1]	m^*/m_0 this exp.	m^*/m_0 exp. [4]
$\zeta \langle 110 \rangle$	72.3	72.9	73	1.70	1.66
$\zeta \langle 100 \rangle$	82.7		80		
$\zeta \langle 111 \rangle$	62.2	62.3	61	1.52	1.52
$\epsilon_2 \langle 110 \rangle$	4.05	4.11		0.39	0.28
$\epsilon_1 \langle 110 \rangle$	3.60	3.68	3	0.22	0.24
$\epsilon_{1,2} \langle 111 \rangle$	3.62	3.61		0.23	0.26
$\gamma \langle 110 \rangle$	0.55		0.7	0.19	
$\gamma \langle 100 \rangle$	0.35	0.37		0.11	
$\beta \langle 110 \rangle$	0.33		0.4	0.11(4)	

3. **Energy band calculations.** — The energy band calculation for LaAl_2 [1] is based on the nonrelativistic augmented plane wave (APW) method using the atomic starting configuration (4f 5d 6s) for the La. In figure 2 we show cross sections through the Fermi surface tentatively extracted from those energy bands. There is a large Γ -centered electron surface, the extremal areas of which are in good agreement with the experiment (ζ -oscillations). Probably there are small holes around X, L and W corresponding to flat energy bands at E_F . According to the component density of states calculations [1] the 4f-like states in La contribute through hybridization about 1/3 to the total density of states at E_F . Those smaller areas are therefore more sensitive to 4f-like contributions than the larger Γ -centered areas resulting from steep energy bands at E_F . The agreement between experiment and theory for the ζ -oscillations is thus not so surprising.

4. **Conclusion.** — Based on our measured dHvA oscillations and the non self-consistent non relativistic APW energy band calculation [1] a Γ -centered large

Fig. 2. — Cross sections through the Fermi surface of LaAl_2 tentatively deduced from energy band calculations [1],

$$(2\pi/a)^2 = 62.33 \times 10^6 \text{ G}.$$

electron Fermi surface can be well established. It is essentially spherical but with bumps in $\langle 100 \rangle$ directions. Two more groups of lower dHvA frequencies have been detected and several effective cyclotron masses have been measured, however, it is rather speculative to construct further small (hole) surfaces based on [1]. Self-consistent calculations would change the f character of La bands and might shift the La bands with respect to the Al bands. Furthermore, the inclusion of spin-orbit coupling would remove some degeneracies. Thus unless more refined energy band calculations are available (including cyclotron masses) the interesting question how the nearby La f-band affects the electronic properties of LaAl_2 cannot be answered satisfactorily. More detailed experimental results on LaAl_2 including Dingle temperatures and a comparison with dHvA effect measurements in YAl_2 will be given later [5].

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