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FERMI SURFACES AND EFFECTIVE MASSES IN LnB_6 , $\text{Ln} \equiv \text{La}$, Ce AND Pr^*

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Summary

The Fermi surface has been compared for the three compounds LnB_6 ($\text{Ln} \equiv \text{La}$, Ce and Pr) by measurement of the de Haas-van Alphen effect. The major part is observed to be similar in each compound, most likely consisting of X-centred ellipsoids with a total effective volume of about 1 electron per formula unit. Differences occur in the details of the shape of the FS, clearly seen for PrB_6 .

Large effective masses, m^* , are observed for CeB_6 and PrB_6 , $m^* = 6$ and about 1.8, respectively. These have to be compared with $m^* = 0.6$ for LaB_6 .

Introduction

In metallic lanthanide systems many questions arise around the character of the 4f electrons, being localised on the ion core or assuming an itinerant character, through the formation of bands hybridised with the s and d states. From the experiments direct information can be obtained by studying Fermi surfaces (FS), their shape and derived properties, and comparing the FS for several Ln compounds of similar nature. When hybridisation takes place one expects to find large dissimilarities.

One such system has been investigated earlier by Johanson *et al.* [1]. From data obtained by the de Haas-van Alphen effect (dHvA) they concluded on large differences between the FS of LaSn_3 and CeSn_3 . In both compounds orbits are observed which belong to parts of the FS enclosing a substantial part of the Brillouin zone (BZ) volume, *i.e.*, containing a large number of electrons. From the very observation of such orbits they conclude

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that the behaviour of the electron states is coherent over several hundreds of unit cells.

The FS of LaB_6 has been the subject of earlier investigations [2, 3]. Experiment (dHvA) and band theory agree on an FS having a total volume of one electron per formula unit, consisting of large, X-centred electron ellipsoids. The ellipsoids are interconnected by necks along the X-X directions; orbits around the necks and on the ellipsoids crossing the necks are observed over a limited angular range for directions around [100].

Results and Discussion

Here we report data on the shape of the FS for other LnB_6 compounds. The experimental procedure has been described elsewhere [4, 5]. The dHvA oscillations are detected in high magnetic fields, between 10 and 21 T for LaB_6 and PrB_6 , respectively, 25 and 33 T for CeB_6 , at temperatures between 1.3 and 4.2 K.

CeB_6 shows several magnetic phases as functions of temperature and field [6, 7]; one infers from the magnetisation data that in the region where dHvA is measured, a ferromagnetic ordering is imposed by the magnetic field. For PrB_6 the situation is less clear. From neutron scattering it was found [8] that two magnetic structures exist in zero field, a commensurate antiferromagnetic for $T < 4.2$ K and an incommensurate for $4.2 \text{ K} < T < 6.9$ K. The moment at $T = 1.74$ K is $1.77 \mu_B$. We measured the magnetisation on a sample consisting of a large number of single crystals. At a temperature of 4.2 K it varies approximately linearly with magnetic field up to 15 T; at 15 T one finds $0.7 \mu_B$ per Pr atom.

For LaB_6 , dHvA frequencies are obtained as given earlier by Arko *et al.* [2]. Our results for the Ce and Pr compound are given in Fig. 1. For PrB_6 the labels are given based on the merging of branches at high symmetry directions, indicating that the corresponding surfaces are connected through symmetry. For CeB_6 the labels are attributed based on the similarity to PrB_6 .

In all three compounds dHvA orbits are observed with frequencies ranging from 8 to 10×10^3 T, labeled "a" in Fig. 1. For LaB_6 they are the belly orbits on the X-centred ellipsoids, χ in the notation of ref. 2. In a comparison of the a-branches in Fig. 1 with the data for LaB_6 (ref. 2), a striking similarity is seen. For PrB_6 and LaB_6 the frequencies are nearly equal; for CeB_6 they are 5 - 10% larger. The data for the Ce compound do not extend over the full (110) plane for experimental reasons rather than for the non-existence of dHvA orbits near [110].

For PrB_6 two other sets of branches, labeled "b" and "c" are observed. Most of them are detected over the full (110) plane, indicating that the corresponding FS sheets are closed. This is in contrast to the LaB_6 case, where the lower frequencies are due to orbits involving the X-X necks. The three-fold degeneracy of the b branches for the [111] orientation may have two causes; it can be due to a non-symmetry position in the BZ of the centre of

Fig. 1. Observed de Haas-van Alphen orbits in the (001) and (110) planes for CeB_6 and PrB_6 . The ordinate is in units of 10^3 Tesla. The orientation dependence of the high-frequency branches labeled a is similar to the one observed for LaB_6 . The labels a, b, and c, are used with suffixes, based on the merging of the branches at the high-symmetry orientations only.

the corresponding sheets. In addition, it may stem from exchange splitting between the two spin directions. However, no such splitting is unambiguously resolved for the other sheets.

The effective mass, m^* , of the a branches has been determined by fitting the temperature dependence of the dHvA amplitude to the Lifshitz-Kosevich [9] expression. In PrB_6 we find m^* equal to 1.9 ± 0.2 and 1.8 ± 0.2 for $a_{1,2}$ and a_3 , respectively, for the [001] orientation, using five temperatures between 1.3 and 4.2 K. No such accuracy is obtained in the case of CeB_6 , as the signal is only observed for temperatures between 1.3 and 2.2 K. The value obtained is 6 ± 2 for the a_3 branch along [001]. For LaB_6 the corresponding values are 0.65 and 0.61, respectively [2].

The a-branches shown in Fig. 1. have the highest frequency which varies only 25% over all orientations; they stem from orbits on the major FS sheets. When the a-branches have a common origin, the threefold degeneracy in the (001) plane places the centre of the sheets at the X point in the BZ, or M. The dominant part of the Fermi surfaces then has a strong similarity to the one of LaB_6 . In this picture the f electrons are localised; they influence mainly the dispersion at E_F , increasing the effective masses above the value for LaB_6 . The b- and c-branches for PrB_6 may arise from distortions of the LaB_6 bands near E_F . No obvious explanation is available for the a' branch.

Conclusion

A direct interpretation of the FS data in terms of a band structure is not yet possible due to the lack of a sufficiently detailed calculation, allowing

for the magnetic structure of the materials. A nonmagnetic calculation has been carried out, treating the 4f electrons as itinerant for CeB₆ [10] and for CeB₆ and PrB₆ [11]. Both calculations indicate 4f states close to E_F and strongly mixed with the boron-derived band that is responsible for the Fermi surface of LaB₆. The FS derived for the heavier Ln compounds do not resemble the one for LaB₆ at all. It is made up of sheets centred at Γ and R; their size is of the correct order of magnitude when compared with the a-branches. In this case the similarity between the three compounds is incidental. A comparison with the refined calculation will provide a better answer.

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