PHYSICAL REVIEW B **67**, 012405 (2003)

Elastic anomaly in Tb under uniaxial tension: Evidence of the change in the Fermi surface topology responsible for the magnetic ordering type

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(Received 26 June 2002; published 24 January 2003)

A single crystal of Tb was examined under uniaxial tension applied along the hexagonal axis by a x-ray dilatometry and resistive strain sensors. The experiment was carried out well above the magnetic ordering temperature. The strain-stress dependencies obtained exhibit the characteristic violation of linearity that is evidently due to the change in the Fermi surface topology caused by strain. This electron-topological transition is presumably responsible for the recently observed change in the magnetic ordering type in the same sample.

DOI: 10.1103/PhysRevB.67.012405 PACS number(s): 75.25.+z, 71.18.+y, 75.30.Kz, 75.50.Ee

I. INTRODUCTION

Heavy rare-earth hcp metals are believed to be materials in which the fine structure of the Fermi surface (FS) directly determines the type and the properties of the magnetic structure. That is one of the reasons why the FS in these metals, in itself rather complex and intriguing, has been attracting special attention for a long time.

The magnetic structures in these materials possess a huge variety of properties. The helical, sinusoidal, cycloid, fan, etc., periodic structures occur under different circumstances. These complex magnetic structures are all characterized by a long period, i.e., its magnetic wave vector q, always directed along the hexagonal axis, is about an order smaller than the Brillouine zone size.

It was suggested more than 30 years ago[1] that this wave vector value is determined by nesting phenomenon, first proposed for chromium by Lomer[2] and extended to rare-earth metals by Dzyaloshinski.[3] According to this hypothesis, the magnetic wave vector q is exactly equal to a certain extreme diameter of the FS. This diameter was supposed to be a diameter of the so-called "webbing" feature in the L point of Brillouine zone (see the introduction in Ref. 4 for a detailed description). Presently this concept is commonly accepted.

The classical calculations of the FS in rare-earth metals[1] revealed that the FS shape depends strongly on the initial parameters. Particularly, the calculated FS of Tb, Ho, Dy, Er, Y exhibit the above-mentioned webbing feature, while there is no such feature in the FS of Gd. The further investigations of the FS in these materials[4–9] never affected the main conclusions. The two plausible topologies of the FS are presented on Fig. 1. These sketches summarize Refs. 1, 4 and 9 The "yttrium-type" topology presented on Fig. 1(a) is believed to provide complex periodic magnetic structures (nesting vector q indicated by arrows), while the "gadolinium-type" topology in Fig. 1(b) corresponds to the simple ferromagnetic ordering characteristic for Gd and Gd-rich alloys.

In Ref. 10 we emphasized that all these materials, being closely related, are hence in the vicinity of change in the FS topology. Thus the shape of the FS in these materials might be easily changed by external action. The most effective way to change the FS shape is to apply the uniaxial tension/compression that changes the c/a ratio of the crystalline lattice parameters since this ratio is the primary parameter that determines the FS shape in the hcp metal. Considering the yttrium-type FS like that of Tb, one can expect its conversion to the gadolinium-type under uniaxial tension (see below). If occurs, this change would be an example of the electron-topological transition, alias Lifshitz transition or $2\frac{1}{2}$ type transition.[11] According to the nesting hypothesis, such a transition shall be accompanied by a change in the magnetic ordering type.

The electron-topological transition is a phenomenon associated with the qualitative change in the FS geometry under variation in some parameter, such as temperature, pressure, or chemical content. The proposed evolution of the FS of Tb under uniaxial tension p is sketched in the inset Fig. 3: the

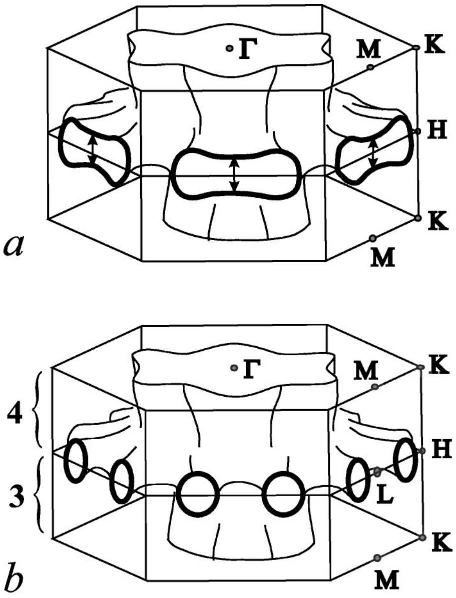

FIG. 1. Two plausible topologies of the Fermi surface in heavy rare-earth metals (double zone presentation, semiquantative sketch): (a) A webbing feature is present (indicated by bold line), complex periodic magnetic ordering expected. Arrows mark the extreme diameter responsible for nesting, that is presumably equal to the magnetic wave vector q. (b) No webbing feature, simple ferromagnetic ordering expected. Zones labeled by numbers. The possible "arm" in M point is not presented.

two opposite surfaces of the above mentioned webbing feature contact each other, hence forming a neck. According to the theory Refs. 11 and 12 the nesting vector *q*, elastic moduli c_{ij}, resistance *R*, density of states on the Fermi level $n(e_F)$, and specific heat *C* shall all follow the square-root dependence on tension $\propto(p^* - p)^{1/2}$ in the vicinity of the electron-topological transition, where p^* corresponds to the transition. This term exists only when webbing feature is present, i.e., at $p < p^*$. The square-root dependence of this sort is the signature of the Lifshitz transition. Typically this contribution is added to the ordinary regular behavior, hence the relative size of the phenomenon can be hardly estimated *a priori*.

Our experiments[13,14] confirmed that the change in the type of the magnetic ordering under uniaxial tension/compression might in fact occur. We associated this change with the change in the FS topology under deformation. Nevertheless this proposed electron-topological transition shall only be treated as speculation, as it was merely deduced from the change in the magnetic properties and was never confirmed directly. To complete the framework it is necessary to obtain nonmagnetic evidence of the electron-topological transition under elastic strain. This is the goal of the present study. We expected to observe the square-root dependence of the elastic moduli of Tb on the uniaxial tension as evidence of the Lifshitz transition.

II. EXPERIMENT

In our recent work[14] we have demonstrated that the uniaxial tension applied to a single crystal of Tb along the hexagonal *c* axis suppresses completely the originally antiferromagnetic helical ordering at the Néel temperature in favor of simple ferromagnetic ordering. The critical tension value, presumed to correspond to the change in the FS topology, was $p_c = 680$ bar.

In the present experiment we examined the same sample in the same experimental cell under uniaxial tension at room temperature 293 K, i.e., far above the magnetic ordering temperature (231 K in our case). The magnetic phenomena at this temperature might be completely neglected; hence the elastic anomaly, if it occurs, can be due only to the conducting electrons responsible for the chemical bond, i.e., to the FS features.

For the description of the sample and the experimental cell see Ref. 14. To obtain the crystalline lattice parameters we used two experimental techniques: x-ray dilatometry, which gives the exact lattice parameters, and resistive strain sensors, which are more sensitive but less direct. These measurements were carried out independently.

The x-ray experiment was carried out on a Rigaku Geigerflex diffractometer using a $K\alpha$ doublet of Co. The high-angle (300) and (205) reflections were used to obtain *a* and *c* values. The estimated relative accuracy of the lattice parameters obtained is $\sim 10^{-4}$ with probable regular shift also within $\pm 10^{-4}$. The load applied to the sample was produced by the calipered spring. The cell temperature monitored by thermocouple remained the same within ± 0.3 K during the experiment.

The two almost equal resistive strain sensors of initial resistance $R = 152.3$ and $152.4\,\Omega$ had the operating size of 2.5×1 mm^2. Its sensitivity is $\Delta R/R = 2.05\Delta l/l$, where *l* is the size in the operating direction. These sensors were glued onto the opposite faces of the sample parallel and orthogonal to the *c* direction respectively. We used the rigid phenol-aldehyde glue (Russian-made BF-2) subjected to thermal polymerization.

To obtain the $\Delta a/a$ and $\Delta c/c$ tension dependencies, the respective sensor was switched into the ordinary resistive bridge that provided sensitivity of $\Delta R/R \approx 10^{-6}$. We also obtained independently the $\Delta(c/a)/(c/a)$ tension dependence when these two sensors were switched into the opposite arms of the resistive bridge. The accuracy estimated by comparison of these three dependencies is some $\sim 10^{-5}$.

These sensors appeared to be sensitive to the parasitic rotative stresses inevitable if the load is produced by spring. Hence we had to use a less disturbing way of loading. Following the ancient experimental style, the load was produced by the weight of a vessel gradually filled by water. This way appeared to be convenient and provided the well reproduced strain-stress dependencies. All the dependencies were reproduced repeatedly; hence the tension applied caused no irreversible deformations.

To ensure the absence of the mechanical effects such as friction or wedging that could affect the load transmission to the sample, we mounted another resistive strain sensor directly on the beryllium-copper sample holder and obtained the strain-load dependence for this holder. This dependence was well linear, the mechanical hysteresis being negligibly small. Hence the load applied to the sample was confirmed to be equal to the known load applied to the experimental cell. The tension value was calculated directly as the load applied divided by the sample crossection. The tension never exceed 800 bar due to fear of the sample rupture.

III. RESULTS

The x-ray experiment confirmed that the crystalline lattice remains hcp under all the tensions applied. No broadening of the reflections with tension was observed. The tension dependencies of the lattice parameters *a* and *c* are presented on Figs. 2(a) and 2(c), respectively. The *c/a* ratio obtained from these data is presented in Fig. 2(e).

The tension dependencies of the strains measured by resistive sensors mounted along *a* and *c* directions are presented on Figs. 2(b) and 2(d), respectively. The dependence for c/a, obtained independently as described above, is presented in Fig. 2(f). Vertical scales for these plots were adjusted so that the same change in the parameter is reflected by the same vertical shift on both the x rays and resistive plots for this parameter. As the x-ray beam illuminates a certain point of the sample's surface, while the strain sensor averages the strains over all the sample's face, some discrepancies could be expected. Nevertheless the curves obtained by different techniques demonstrate the agreement within the experimental accuracy. The dashed lines present the change in the respective parameter with tension calculated in the linear approximation using elastic moduli values.[15] The

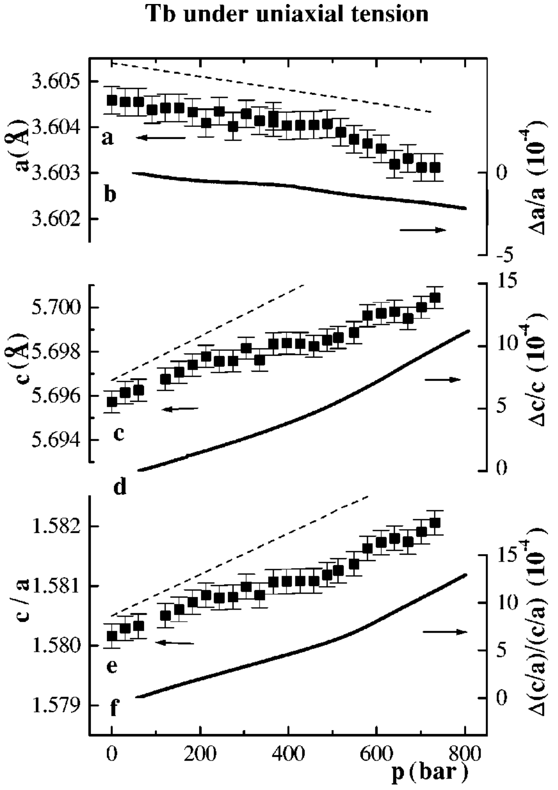

FIG. 2. Tension dependencies of the lattice parameters. (a),(c) x-ray data for a and c. (e) c/a ratio obtained from (a),(c). Panels (b), (d), (f): relative changes in a, c, and c/a ratio respectively, obtained by strain sensors. Dashed lines present the same dependencies in the linear approximation (see text).

agreement with our results at low tensions is good, which confirms the validity of the measurements.

The violation of the Hooke's law at tension $p^* \approx 600$ bar is clear on all the plots for c and c/a. According to the theory (see above) the elastic modulus shall exhibit the characteristic contribution, square-root dependent on the tension applied, at $p < p^*$.

To separate this contribution we obtained the numerical derivative of the most pronounced curve, Fig. 2(d). The result, actually the reciprocal sample rigidity, is presented in Fig. 3. The dashed curve is a square-root fit (with the linear onset). Both the negative square-root contribution below the critical tension p^* (marked by arrow) and the exactly linear dependence above this tension, in complete agreement with the theoretical expectations, are obvious. The change in the sample rigidity is surprisingly pronounced. The extrapolation of the fit never gives intolerable negative values. The critical tension value p^* that corresponds to the kink is equal to 650 bar. The respective critical $a,c,c/a$ values are 3.6040 ± 0.0005 Å, 5.700 ± 0.001 Å, 1.5818 ± 0.0003.

IV. CONCLUSIONS

In our recent work[14] the critical tension p_c, which corresponds to the change in the magnetic ordering type in Tb, was found to be 680 bar. In the present experiment carried out on the same sample the critical tension appeared to be 650 bar. Such an agreement can be called equality beyond any reasonable doubt. It was hence demonstrated that both the change in the magnetic ordering type and the elastic anomaly in the non-magnetically ordered phase of Tb under uniaxial tension are manifestations of the same phenomenon.

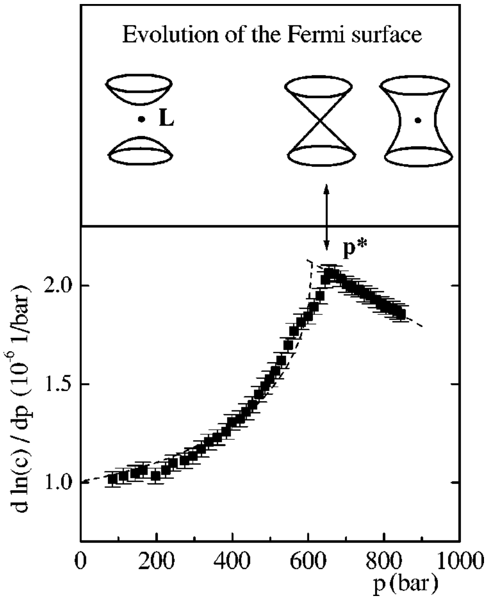

FIG. 3. Pressure derivative of the strain along c axis [from data Fig. 2(d)], proportional to the sample reciprocal rigidity. The dashed curve is a square-root fit. Arrow marks the critical tension $p^* = 650$ bar. Inset: qualitative sketch of the proposed change in the Fermi surface with tension; enlarged axonometric view of the webbing feature [see Fig. 1(a)]. L is the point of the Brillouin zone.

This phenomenon is plausibly the qualitative change in the Fermi surface shape caused by strain, i.e., the electron-topological transition. Such a transition is evident from the band structure calculations in these metals. The theoretical expectations agree completely with the features observed in the experiment.

The main consequences are as follows. First, terbium appeared to be a metal in which electron-topological transition can be easily observed at room temperature. It offers possibilities to study this phenomenon by itself using the appropriate experimental techniques, such as galvanomagnetic, acoustic, positron annihilation, etc.

Second, the exact crystalline lattice parameters that correspond to the change of the Fermi surface topology in Tb were obtained with a four-digit accuracy. This is a challenge for the band structure calculations in $4f$ metals that can now be verified with high accuracy.

Third, the magnetic structure of the metal was demonstrated to be governed by altering the shape of the Fermi surface caused by strain. This phenomenon, noteworthy in itself, can be considered as an essentially unlinear type of magnetoelastic interaction in metals.

Fourth, the phenomenon requires an elaborate theoretical treatment, since the considerations presented are ratherstraightforward. The correct approach shall consider the self-consistent problem for elastic, conducting, and magnetic systems simultaneously.

Fifth, we obtained strong independent support for the nesting hypothesis and likely a fruitful approach to the magnetism in the heavy rare-earth metals, especially for such highly stressed systems as epitaxial films and superlattices.

ACKNOWLEDGMENTS

We are grateful to O. D. Chistiakov for the crystal provided. We are grateful to M. I. Kaganov and R. Z. Levitin for the useful discussions. We are grateful to Yu. P. Gaidukov and A. S. Markosyan for their help in the experiment. The work was supported by the Russian Foundation for Basic Research Grant No. (N01-02-17639).

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