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FERMI SURFACES FOR dhcp La, Nd, AND Pr: RELATIONSHIP TO MAGNETIC ORDERING AND CRYSTAL STRUCTURE*

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(Received 23 September 1968)

The purpose of this Letter is to report the calculation of the relativistic energy bands and Fermi surfaces of the double hexagonal close-packed light rare-earth elements lanthanum, neodymium, and praseodymium. The relationship of the Fermi surface to the ordering of magnetic moments in Nd and Pr and to the occurrence of the double hexagonal close-packed crystal structure is then discussed.

Although the heavier rare earths have been studied extensively in recent years,[1-4] no calculations have yet been made for the double hexagonal close-packed (dhcp) lighter metals.[5] In addition several investigations have been made relating magnetic ordering and Fermi-surface effects in transition and heavy rare-earth metals.[6-8] It was originally proposed by Lomer[6] that the wave vector separating two flat pieces of Fermi surface corresponds to the periodicity of the ordering of the magnetic moments in chromium. Keeton and Loucks[4] have observed that in the heavy rare-earth metals there is good agreement between the magnetic-ordering wave vector and the Fermi-surface separation. This was verified analytically in the recent susceptibility calculations of Evenson and Liu.[8] For Nd and Pr complex magnetic structures have been observed[9,10] which should be related to features of the Fermi surfaces of the two elements.

The energy bands were calculated using the relativistic augmented-plane-wave method developed by Loucks.[11] This method is a relativistic generalization of the augmented-plane-wave (APW) method proposed by Slater[12] and has been previously used for calculation of the electronic structure of the heavy rare-earth elements.

The dhcp unit cell consists of four atoms located at $(0,0,0)$, $(\frac{1}{3},\frac{2}{3},\frac{1}{4})$, $(0,0,\frac{1}{2})$, and $(\frac{2}{3},\frac{1}{3},\frac{3}{4})$, where (p,q,r) means $p\vec{a}_1+q\vec{a}_2+r\vec{a}_3$ and $\vec{a}_1=a\vec{i}$, $\vec{a}_2=\frac{1}{2}a\vec{i}+\frac{1}{2}\sqrt{3}a\vec{j}$, and $\vec{a}_3=c\vec{k}$. The values of the lattice constants a and c used are those given by Pearson.[13] The crystal potential was approximated by a muffin tin potential constructed from a superposition of atomic potentials[14] using the Slater $\rho^{1/3}$ exchange.[15]

The electronic configuration used for La was $5d^16s^2$ while for Nd and Pr the configuration was $5d^06s^2$, which is the free-ion configuration. While the metallic configuration is actually $5d^16s^2$, it has been shown in the heavy rare earths that the difference produces only a small change in the bands.[4] The radius of the APW sphere used was 3.320 a.u. The same 41 reciprocal lattice vectors were used for the wave function expansion at all points in the 1/24 zone. This set of reciprocals was found to give convergence to within 0.002 Ry at the high-symmetry points in the primitive Brillouin zone.

The bands calculated for La along lines of high symmetry are plotted in Fig. 1. The Nd and Pr bands are very similar to those for La and need not be shown at this time.[16] These will be presented in detail in a future paper presenting sus-

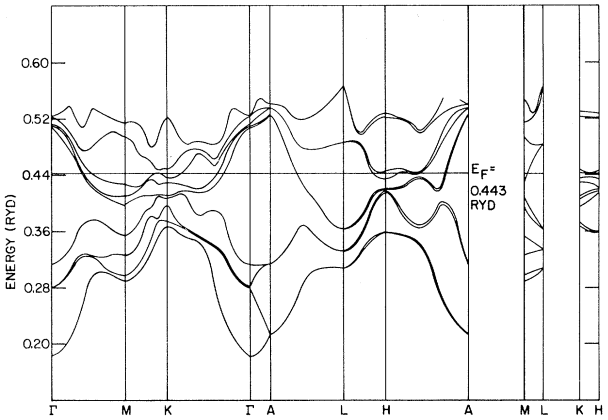

FIG. 1. La energy bands along high-symmetry directions.

ceptibility calculations for Nd and Pr.[17] From these bands the density of states at the Fermi energy has been calculated. These were found to be 19.4, 16.8, and 16.2 states/Ry atom for La, Nd, and Pr, respectively.[18] The only experimental determination of any of these known to the authors was made for La by Johnson and Finnemore[19] who found $N(E_F)$ to be 27.2 states/Ry atom. Recent calculations by McMillan[20] indicate that electron-phonon interaction can account for the difference between this value and that which we have calculated.

The intersections of the La Fermi surface with the faces of the 1/24 Brillouin zone are shown in Fig. 2. The fifth-zone hole surface is a nearly circular cylinder of radius $0.18b_1$,[21] centered along ΓA and indicated by the dark shading on the drawing. There are two small ellipsoids of seventh- and eighth-zone electron surface along AH and KH (crosshatched region). The sixth-zone hole surface is a column along the ΓA axis which tapers from a nearly hexagonal cross section with faces separated by $0.4b_1$ in the ΓKM plane to a circular cross section with an approximate diameter of $0.36b_1$ in the AHL plane. The intersections of this region with the faces of the 1/24 zone are shown as the lightly shaded region in Fig. 2. The surface which we feel is of major interest at the present time is that of seventh-zone electrons (diagonally shaded region). It has a nearly circular cross section near H and then gradually extends out along the $KMHL$ zone face until nearing the ΓKM plane. Then it broadens rapidly towards Γ producing a shelf centered about M in the ΓKM plane.

In Nd and Pr we feel that it is this flat region parallel to the $KMHL$ zone face which will determine the magnetic ordering which has been ob-

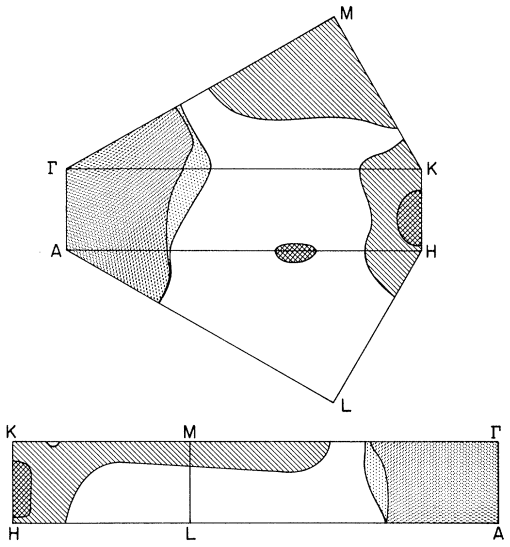

FIG. 2. Intersections of the La Fermi surface with faces of the 1/24 Brillouin zone.

served. Two cross sections of the Nd Fermi surface near this face are shown in Fig. 3 indicating wave vectors which contribute to determining the periodicity of the magnetic ordering. These are taken for z component of wave vector of (a) $\frac{1}{6}b_3$ and (b) $\frac{1}{4}b_3$ corresponding to slices at one-third and one-half the distance from Γ to A. The wave vector $\vec{q}_1$ separates the Fermi-surface regions most responsible for the ordering but additional contributions come from pieces separated by $\vec{q}_2$ and $\vec{q}_3$.

In contrast to the heavy rare earths where the magnetic-ordering wave vector lies along the $\vec{b}_3$ axis, the ordering for Nd and Pr is along the $\vec{b}_1$ direction and has a periodicity corresponding to a wave vector of magnitude $0.13b_1$ at the Néel temperature.[9,10] It is significant that our Fermi surface indicates that the ordering should occur along this direction, and a first estimate based on the seventh-zone electron surface indicates a wave vector ($\vec{q}_1$) of about this magnitude for the magnetic ordering. Detailed calculations of the magnetic susceptibility are now being made which will include contributions from the entire Fermi surface and these will be presented in the near future.[17]

A possible explanation of the occurrence of the dhcp crystal structure for these metals can also be deduced from our results. In the heavy rare earths there are very flat pieces of Fermi surface perpendicular to the c direction.[1,2,4] These occur about half-way between the center and the edge of the Brillouin zone. If there exists in the

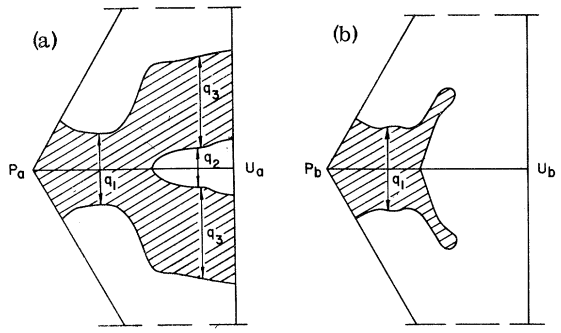

FIG. 3. Cross sections of the Nd Fermi surface near the *KMHL* zone face for (a) $k_z = \frac{1}{6}b_3$ and (b) $k_z = \frac{1}{4}b_3$.

crystal a periodic potential with a period along the c direction equal to twice the lattice periodicity, these flat pieces will be eliminated and the total energy will be substantially reduced. We argue that La, Pr, and Nd take advantage of this situation by going into dhcp structure, and thereby creating just such a potential. Our calculation shows that these flat pieces of Fermi surface are indeed absent in these metals. Therefore, the stability of dhcp over hcp structure is again a consequence of Fermi surface nesting.

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*Work performed in the Ames Laboratory of the U. S. Atomic Energy Commission.

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