TABLE I. Effect of pressure on volume and lattice parameters of magnesium.

P (kbar)	V/V_0	c	a	c/a
0	1.000	5.199	3.203	1.623
25	0.933	5.032	3.145	1.600
50	0.890	4.954	3.096	1.600
75	0.858	4.899	3.057	1.603
100	0.831	4.862	3.019	1.610
125	0.810	4.848	2.986	1.624
150	0.787	4.808	2.954	1.627
175	0.765	4.763	2.926	1.628
200	0.747	4.730	2.902	1.630
225	0.733	4.718	2.879	1.639
250	0.721	4.713	2.857	1.650
275	0.710	4.711	2.836	1.661
300	0.700	4.710	2.815	1.673

would be a lowering of the Fermi energy accompanying an overlap between the Fermi surface and the Brillouin zone wall. This theory was extended by Goodenough,[7] who pointed out that there could be attractive interaction between the Fermi surface and the zone boundary where they approached without overlapping, and that this interaction could affect the axial ratio and the axial compressibility.

Recent studies indicate that the picture based on a spherical Fermi surface is oversimplified. The calculations of Reitz and Smith[8] and the elastic constant measurements of Smith and his colleagues[9,10] showed that the Fermi surface must overlap the wall of the third Brillouin zone in pure magnesium at one atmosphere.

The detailed calculations of Falicov[11] indicate that the Fermi surface is very complex with a hole in the shape of a twelve-tentacled "monster" in the first and second zone, and electron pockets penetrating in the third and fourth zone in a number of spots including the plane perpendicular to the [002] axis.

In spite of the oversimplification involved in assuming a spherical Fermi surface, many of the qualitative arguments of Jones and Goodenough are almost certainly valid.

The discussions of Jones and of Goodenough give a particularly straightforward picture of the events between say 50 and 200 kbar. It should be kept in mind that compression of the c axis corresponds to expansion of the {002} face of the Brillouin zone. From 20–70 kbar c/a is substantially constant and the resistance decreases in a "normal" fashion. Beyond 70 kbar, a further compression of the c axis (expansion of the [002] axis) would result in extension of the second zone to envelop some of the Fermi surface originally in the third zone. As Jones has shown, this would involve an increase in energy, so the lattice distorts to prevent this

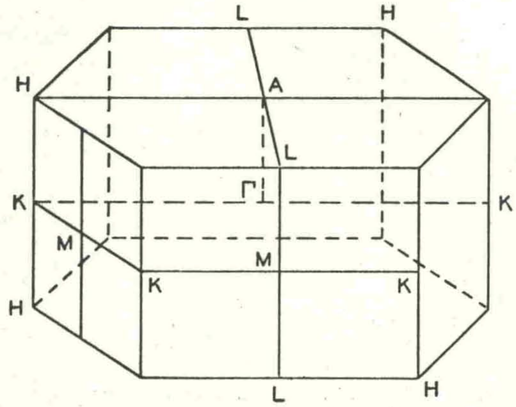

FIG. 7. Brillouin zone for hcp structure with certain symmetry points indicated.

overlap. Thus, c is relatively incompressible and c/a increases. Beyond 120 kbar it costs so much energetically to distort the lattice further that it is preferable to expand the {002} face and overlap part of the pocket of the Fermi surface back into the holes of the second zone. This, however, reduces the number of available conduction electrons. Accordingly, the resistance increases. In the region of highest pressure the c axis is again becoming incompressible, and c/a is increasing, quite possibly due to the approach of the {002} zone boundary to another piece of the Fermi surface.

Some qualitative observations can be made concerning the relationship of c/a ratio to Falicov's calculated Fermi surface. Figure 7 shows the hcp Brillouin zone with certain symmetry points marked using the usual nomenclature. Falicov's calculations show electron pockets in the third and fourth zones at Γ, at L, and at K. The holes in the first and second zone overlap the zone boundaries at H. In addition, the electron pocket at K approaches very closely the hole in this region. A discussion with Dr. Falicov[12] indicates the following qualitative features. (1) A decrease in c/a will be accompanied by decreases in the pockets at L and Γ, a shrinking of the hole at H, and an increase in size of the pocket at K. (2) An increase in c/a will be accompanied by an increase in the pocket at L and a decrease in the pocket at K. The increase in resistance in the region beyond 100 kbar can be accounted for by a decrease in total Fermi surface, quite possibly due to overlap between holes and electron pockets at the point K.

In essence, this last paragraph is a more specific rephrasing of the generalizations based on Jones' theory in terms of the Fermi surface of Falicov.

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