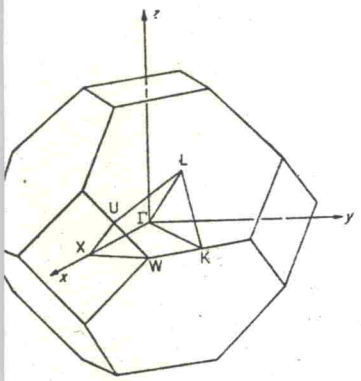
ention on the γ cross-section
is the extremal orbit around
in zone is illustrated in Fig.
ns to the area of this cross-
we must look at the E–k



ce of Al. (From Melz, 1966b.) (b).
wing labelling of some symmetry

t U. The general form of the
ietry directions as calculated
10. The general form of these
e electrons but with certain
ie weak pseudo-potential.
around U and our attention
(U_3); in particular on whether
i level is also indicated in the

the applied magnetic field in
the corresponding extremal
(Fig. 10). On going from U
E–k curve reaches the Fermi
s X (the centre of the square
mi level at B.
given by:

$$E_{U_3} = T_U + \frac{1}{2}\{V_{200} + (V_{100}^2 + 8V_{111}^2)^{\frac{1}{2}}\} \qquad (32)$$

where T_U is the free-electron kinetic energy at U. The coefficients V_{200} and V_{111} have been referred to above; they may be thought of as Fourier components of the lattice pseudo-potential or as matrix ele-

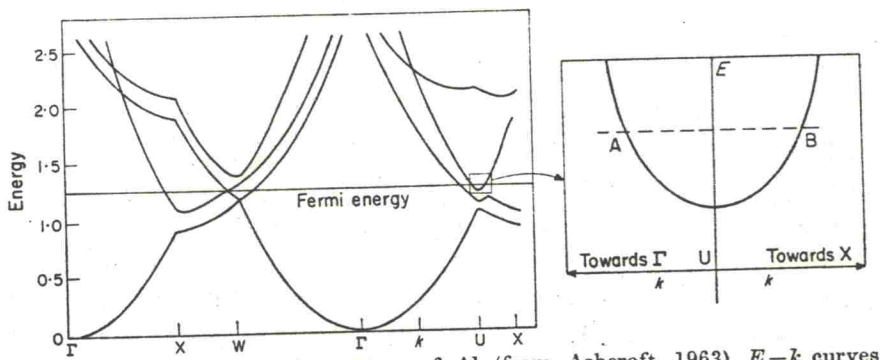


FIG. 10. Calculated band structure of Al (from Ashcroft, 1963). $E-k$ curves in the neighbourhood of the point U.

ments of the pseudo-potential taken between 2 orthogonalized plane waves differing by the reciprocal lattice vectors (200) and (111), respectively. V_{200} and V_{111} are positive. Moreover, Harrison (1965) has estimated that the pseudo-potential coefficients for Al should increase when the metal is compressed. Consequently, E_{U_3} would increase further above the free-electron value. Of course, both the free-electron kinetic energy and the Fermi energy would increase on compression, but these changes are small compared to the change in E_{U_3} (i.e., the energy splitting due to the pseudo-potential). The final result is that the whole third band is raised with respect to the Fermi energy and so, provided that the band retains its shape, the Fermi surface cross-section, γ (measured by the distance A–B in Fig. 10), will decrease under pressure.

To make a quantitative calculation of this effect, Harrison's model can be used in the manner indicated above to calculate the changes in the pseudo-potential due to pressure.

Melz carried out these calculations and found that a higher-order correction, arising from the next two higher energy levels, has a significant effect on the result. This higher-order effect can be put in without introducing new parameters. His results are shown in Fig. 11, and can be