

boundaries. Likewise in Li, large and comparable to that in K the Fermi surface is still very close to a sphere; Rb, the distortion amounts (Mara and Templeton, 1965) to (Ham, 1964) the Fermi surface is distorted; these indicate a

We see, therefore, that the interaction among the alkali metals, is not too close. One might, therefore, expect a pressure dependence: i.e., that the Fermi surfaces of Li and K are not too far from being spherical. It is likely that the Fermi surfaces of Li and K will change under pressure. The influence of pressure on these two metals is not clear. However, Ham's calculations have shown that changes of resistivity under

implies that the surface must bulge out in some other directions. Because of the energy gap at the [111] zone faces and because these faces lie close to the undistorted Fermi sphere, the Fermi surface tends to bulge towards these faces. This, together with the [110] concavities, forces the Fermi surface actually to contact these [111] zone faces. It is significant that the area of contact is greatest in Cu, which has the highest d levels, next greatest in Au and least in Ag, which has the lowest lying d levels.

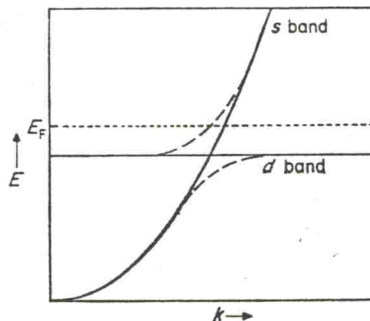


FIG. 15. The effect of interaction between s and d bands (schematic).

surface of Cu at atmospheric pressure. The low-lying fully occupied d bands are. Segall emphasized that the energy of the sp energy bands depends on the direction of compression. It is particularly strong that if the Fermi level lies near that of the d levels, the effect of pressure on the Fermi surface of the s like electrons in noble metals tends to be pushed towards the concave areas around the [110] directions, particularly conspicuous in Au and Ag. In Cu, one electron per unit cell has a Fermi surface, this inward bulging

On this basis one may conjecture that the influence of pressure on the Fermi surface of the noble metals will make itself felt most strongly through the d electrons. On compressing the metal, the d bands would be expected to broaden in energy, and their mean energy to rise.† This will increase the effects of the interactions between sp like and d like energy bands, which in turn would exaggerate the distortion already referred to. Consequently one would expect that pressure would increase the areas of contact in the [111] directions and enhance the concave areas in the [110] directions. The experimental results of Templeton show that, at least as far as [111] directions are concerned, these ideas correspond with what is found experimentally. There have recently appeared some calculations of the effect of volume change on the Fermi surface of copper by Davis *et al.* (1968).

† A rough argument is as follows. Compressing the metal increases the overlap of the original atomic d orbitals. Consequently the d band will broaden on compression. A rise in the average band energy may be attributed to the increase on compression of the exponentially varying repulsion between the closed shells.