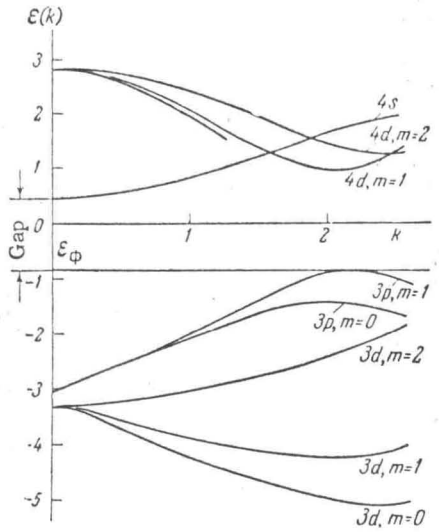

which would fill the levels with n = 1, 2, and 3 if the level distribution were hydrogen-like; nickel would then be an inert gas. In fact, under normal conditions in the metal, the 4s-band is lower than the 3d-band. Due to electron transitions from 3d to 4s we have the unfilled bands responsible for conduction. On increase of the density the level 4s rapidly rises and becomes higher than the levels 3s, 3p and 3d. We then have the situation when all the bands with $n \leq 3$ are filled and nickel becomes a dielectric. At still higher densities we can expect overlapping of the 3p and 4d bands, making nickel again a metal (for $\delta > 15$, $\rho > 130$ g/cm^3, $p > 1500 \times 10^6$ atm).

The bands calculated for $\delta = 8.56$ are shown in the figure, which gives the dependence of the energy (in atomic units) on the wave vector of the electron.[1)] The spectroscopic index of the electrons is given for each branch and this index includes the magnetic number m which is the projection of the magnetic moment along the direction of the momentum k.

Caution is needed in calculating the critical density, since the calculations are based on the spherical approximation for the quasimomentum k. If the true form of the Brillouin zone for fcc nickel is allowed for, the upper edge of the 3p-band along some directions in k-space may be higher than in the spherical case. It is therefore desirable to estimate the possible increase of the energy maximum for the 3p-band. For this purpose the Slater-Koster interpolation method [2] was used. To find the constants we used the formulas for the energy $\epsilon(k)$ along the most symmetrical direction [010] in k-space. Along this direction the upper edge of the 3p-band was displaced upwards a little to −0.62, but it remained below the lower edge of the 4s-band. Of the remaining directions the most likely to show an energy shift is the direction [111]. Although the spherical approximation is insufficient for finding all the nondiagonal constants in the Slater-Koster technique, it is nevertheless clear that in a wide range of values of these constants there is an energy gap between the 3p-band and the 4s-band.

In connection with the general rule for the transformation of any substance into a metal on unlimited increase of the density, we should note that the decisive factor is the deviation of the unit cell of the crystal (having the form of a polyhedron) from spherical shape. Let us consider a degenerate electron gas in the field of a uniformly distributed positive charge. For this gas $E = k^2/2m$. Replacement of the smeared-out charge distribution by separate ions at lattice sites may be regarded as a perturbation. It is known that in this case the hypersurface $E(k)$ splits up into separate zones divided by gaps. On increase of the density the gap widths decrease but the gaps do not disappear! In this approximation substances with certain values of Z (in particular helium) would remain dielectrics at any density. However, since the unit cell shape is not spherical the limiting momentum depends on the direction with respect to the lattice and the limiting energy in the band depends on the direction of k. Consequently, at high densities the upper edge of the filled band along one direction of k moves below the bottom of the next unfilled band along another direction of k, and the substance becomes a metal in spite of the fact that the gap still remains.

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1)The reciprocal radius of a Wigner-Seitz sphere is taken as the unit vector.

[1] G. M. Gandel'man, JETP 43, 131 (1962), Soviet Phys. JETP 16, 94 (1963).

[2] J. C. Slater and G. F. Koster, Phys. Rev. 94, 1498 (1954).

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