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METALLIZATION OF SOLID ARGON UNDER COMPRESSION

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THE present author is currently investigating theoretically the behavior of various elements under compression, using the solution of the Hartree equation for crystals.

The method of making such quantum-mechanical calculations was described earlier.[1] In an investigation of the behavior of the electron bands of solid argon, it was found possible to observe the metallization of the sample when it is subjected to a compression given by the factor $\delta = 3.2$ (the initial density of the solid argon was $\rho_0 = 1.9$ g/cm^3).

In its normal state, solid argon is a typical atomic crystal whose binding energy is due to van der Waals' forces. The quantum-mechanical method used here does not describe van der Waals' forces. With this method, only the close packed structure of argon is considered and there should be a small pressure at $\delta = 1$. Calculations do indeed give a very small pressure in the initial state at $\delta = 1$. Under subsequent compression, the van der Waal's forces are unimportant and the results from the pressure calculations represent the real situation in the compression of argon. According to those calculations, the pressure (in megabars) is $p = 0.027$ at $\delta = 1$; $p = 0.324$ at $\delta = 2$; $p = 1.062$ at $\delta = 3$; $p = 2.721$ at $\delta = 4$. The rearrangement of the electron bands under compression is of special interest. In the region $\delta < 3.2$, the upper filled band is the 3p-band. It is filled completely and contains six electrons: two electrons in the sub-band $3p_0$, and four electrons in the sub-band $3p_1$ (the latter number is the projection of the moment along the crystal momentum vector). The 3d-band lies higher and has no electrons at all.

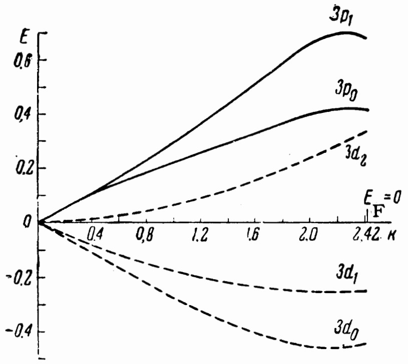

FIG. 1

This state of the crystal is the direct consequence of the well-known state of a free argon atom $(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6$. The experimentally determined excitation energy of the argon atom $(3p)^6 \rightarrow (3p)^5 4s$ is 11.5 eV. The 3d-level in the atom lies close to 4s, but above it. In solid argon, the 3d-band lies below 4s. The present author is not aware of any measurements of the excitation threshold in solid argon. According to our calculations at $\delta = 1$, the gap between the 3p and 3d-bands is equal to 6 eV. Under compression, this gap becomes smaller. At $\delta = 3.2$, the gap is equal to zero and the bands 3p and 3d originate at the same point at $k = 0$ (Fig. 1). (The energy in Figs. 1 and 2 is given in atomic units; 1 atomic unit equals 27.23 eV.) Here, we actually have argon in the metallic state. It is evident from the figure that only the subbands $3d_0$ and $3d_1$, directed downwards, are

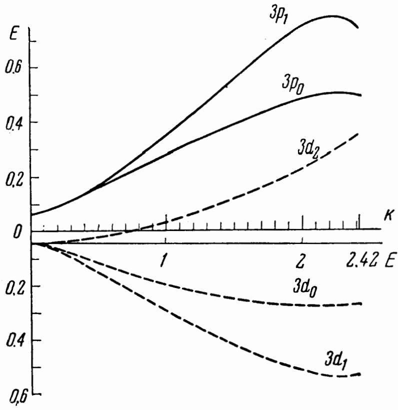

FIG. 2

filled, and the sub-band $3d_2$, shifting upward when the crystal momentum k is increased, is free. It should be mentioned that the sub-bands $3d_0$ and $3d_1$ contain a large admixture of the p-states and are not pure d-bands.

At $\delta > 3.2$, the 3d-band lies below the 3p-band, and the sub-band $3d_2$ touches the sub-bands $3d_0$ and $3d_1$. Figure 2 shows this case for $\delta = 4$. Throughout the region $\delta > 3.2$, we have solid argon in the metallic state with a free sub-band $3d_2$. The pressure at the transition point at $\delta = 3.2$ is 1.29 Mbar at $T = 0$.

Alder and Van Thiel[2] have reported that, at a pressure of about 0.35 Mbar and T = 1 eV, considerable electrical conductivity is observed in a shock wave in liquid argon. If the gap width is of the order of 6 eV, there will be marked thermal electron excitation at 1 eV and the observed conductivity is not surprising. If argon is compressed by two shock waves to 0.7 Mbar and $\delta = 2.5$, then, according to our estimates, the temperature is ≈0.4 eV but the gap width is only 2.4 eV and we can expect considerable electrical conductivity.

The experimental observation of the metallization of solid argon in the predicted range of pressures at low temperatures would be of considerable interest. It would also be very interesting to investigate theoretically and experimentally the features associated with the fact that a free band is in contact with filled bands. In the one-electron Bloch theory, we come to the formal conclusion that the number of free electrons and holes is $n \propto T^{3/2}$ and there is no exponential dependence characteristic of semiconductors. It is not clear how the interaction between electrons and holes may change the theoretical predictions.

The contact at the point $k = 0$ between bands with different l_z applies also in the theory which allows exactly for the lattice symmetry (but not in the Wigner-Seitz approximation).

Since the situation described here occurs over a wide range of pressures, it is possible that this may apply also to another element or chemical compound at normal density, i.e., at zero pressure.

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MAGNETORESISTANCE AND STATIC SKIN EFFECT IN CADMIUM SINGLE CRYSTALS

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THE magnetoresistance of cadmium single crystals, with a resistance ratio $R(4.2^\circ)/R(293^\circ) \approx 10^{-5}$, was measured as a function of an inclined external field when the field dependence was accompanied by the ballistically detected[1] static skin effect.[2] The cylindrical samples, with an inner channel, differed from those described in[1] by their length (25 mm) and the presence of voltage terminals 6 mm from their ends. The magnetoresistance was measured with a compensation circuit, which included a photoelectric amplifier having a sensitivity of 2×10^{-9} V per division of the compensator scale. The angle between the axis of a sample and the magnetic field was 84°.

Figure 1 shows the results of the ballistic $(\Delta\Phi/\Delta\Phi_0)$ and resistometric $[H^2/(R(H) - R(0))]$ measurements, where $\Delta\Phi$, $\Delta\Phi_0$ are the changes in the magnetic flux due to the current in the core of a sample, situated, respectively, in a field H and in the terrestrial magnetic field; R(H), R(0) are the magnetoresistances in the same fields. The observed tendency for curve 1 to approach the origin of coordinates indicates the presence of a linear term in the dependence R(H) in the same range of fields (0-800 Oe), where the ballistic measurements show the process of re-

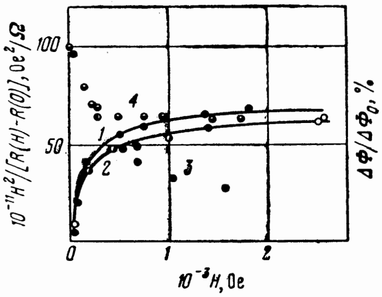

FIG. 1. Results of the ballistic (curves 3 and 4) and resistometric (curves 1 and 2) measurements on cadmium single crystals. Curves are given for samples with smooth (1, 3) and damaged (2, 4) surfaces. Notation: ● – curve 1; ○ – curve 2; ◐ – curve 3; ◒ – curve 4.