SUPERCONDUCTIVITY INDUCED BY PRESSURE

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It has been known recently that certain metals (Cs, Ba, Y, Ce), located in the lower left corner of the periodic table, reveal superconductivity properties at high pressures but not under ordinary conditions [1, 2]. The reason for this phenomena still remains unclear. In the opinion of [2], the pressure-induced superconductivity in these metals is "due to the form of the potential of the ion."

The purpose of the present paper is to attempt to explain the pressure-induced superconductivity from the point of view of the change of the band structure of the elements under pressure. We shall make use of the results of a numerical calculation of the band structure of different elements as functions of the pressure, details of which can be found in [3]. We also wish to call the experimenters' attention to the fact that superconductivity can apparently occur under pressure also in other metals in the first three groups of the periodic table. In our opinion, the pressure-induced superconductivity can be observed in Rb, Sr, and also in K, Ca, and Sc.

The band structure of metals lying in the first three groups of the periodic table, at weak pressures, is similar in many respects to the energy structure of the free atoms. They are characterized by the presence, besides the s-band, of also d-bands in the first group and partly filled d-bands in the second and third groups. For example, these are the 4s- and 3d-bands in Ca, 5s and 4d in Sr, and 6s and 5d in Ba. With increasing number of the group, the occupation number of the d-bands increases. Ce and other lanthanides differ in that they have a partly filled f-band.

With the increasing pressure, the band structure of these metals undergoes the following significant changes. As the compression is increased, the d-bands that lie above the Fermi surface at normal pressure begin to drop and fall on the Fermi surface. In turn, the s-bands rise and approach the d-bands, so that in some pressure intervals the s- and d-bands overlap. Electronic realignment takes place, such that the electrons go over from the s-bands to the unfilled d-bands. With further compression, the s-band turns out to be unfilled and lies above the d-band.

The pressures at which the electronic realignment takes place depend strongly on the compressibility of the medium and increase with increasing number of the group. In K and Ca, for example, this pressure is 150 - 200 kbar, corresponding to compressions by factors 4 - 5. The table, taken from [3], gives the effective number of the electrons in Ca in different bands, as a function of its degree of compression (δ is the ratio of the density of the compressed medium to the density of the medium at normal pressure). We see that in the case of weak pressure the band filled in the main is 4s, which has 1.9 electrons, while the 3d-band has 0.1 electron (the number of valence electrons in Ca is 2). But at $\delta = 3$ we already have the 3d-band more filled than the 4s-band. At $\delta = 4$, the realignment is completed and all the valence electrons are in the 3d-band.

δ	4s	3d
1,5	1,9	0,1
2	1,5	0,5
3	0,7	1,3
4	0,01	1,99

The electron realignment in other elements is similar, the only difference being that other s- and d- or f-bands take part in it. As to the elements of other groups of the periodic table,