AN ESTIMATE OF AN ELECTRONIC TRANSITION IN BARIUM UNDER PRESSURE

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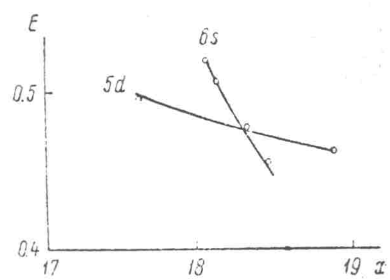
The author and Arkhipov [1] calculated the electronic transitions in cesium and rubidium under pressure using a quasi-classical wave function. The boundary conditions were formulated for the wave function and the dependence of the electron-level energy on the limiting radius of the Wigner-Seitz sphere was calculated. The universal Thomas-Fermi function was used as the potential.

It is very difficult to carry out a similar calculation for elements which have more than one electron in the outer shell, since then one has to allow for the interaction between the electrons in the outer shell. However, if this interaction is simply neglected and the calculation is carried out as for alkali metals, then such a calculation may be used as a rough estimate to check the electronic nature of a given transition under pressure. This calculation has now been carried out for barium under pressure.

An electronic transition in barium may occur on overlapping of the electron shells of 5d- and 6s-electrons. To determine the pressure dependence of the electron-level energy the atomic polyhedron corresponding to each atom in the lattice was replaced by the equivalent Wigner-Seitz sphere of equal volume and the dependence of the energy on the radius of the equivalent sphere was calculated.

The condition which gives the stationary levels of a particle or the lower edge of an energy band in a solid has the following form in the quasi-classical case:

$$\frac{1}{h}\int_0^r p\,dr = \pi(n + {}^1/_2), \qquad (1)$$



Dependence of the energy levels of 6s- and 5d-electrons on the equivalent sphere radius.

where

$$p = \sqrt{\frac{2Z}{\mu}\left[E - \frac{\varphi}{x} - \frac{l + {}^1/_2}{ax^2}\right]}$$

is the "radial momentum"; $\varphi(x)$ is the Thomas-Fermi potential function; E is the energy; and μ is the electron mass. In the earlier paper [1] it was shown that instead of the universal Thomas-Fermi function for a neutral atom, we can use a corrected function for a compressed ion, but since this correction introduced only a small change in the final result it was not made in this case since the result was known in advance to be only an estimate.

The adjoining figure shows the intersection of the energy levels of 6s- and 5d-electrons occurs at the equivalent sphere radius of 18.3 in Thomas-Fermi units or 2.23 A. The equivalent sphere radius for barium at atmospheric pressure is 2.47 A [2]. Thus the radius is reduced by 10%, which corresponds approximately to a 30% change of volume. Using the data on the compressibility of barium [3], we may conclude that the electronic transition pressure lies near 50,000-60,000 atm, which is quite close to the second polymorphic transition in barium.

Concluding, the author regards it as his pleasant duty to thank Corresponding Member of the USSR Academy of Sciences L. F. Vereshchagin for reviewing the work and R. G. Arkhipov for his help.

LITERATURE CITED

1. R. G. Rakhipov and E. S. Alekseev, FTT, 4, 5, 1077 (1962) [Soviet Physics – Solid State, Vol. 4, p. 795].
2. P. Gombas, Statistical Theory of the Thomas-Fermi Atom and Its Applications [Russian translation] (IL, 1951), p. 323.
3. P. W. Bridgman, Recent Work on High Pressures [Russian translation] (IL, Moscow, 1948), p. 71.

All abbreviations of periodicals in the above bibliography are letter-by-letter transliterations of the abbreviations as given in the original Russian journal. *Some or all of this periodical literature may well be available in English translation.* A complete list of the cover-to-cover English translations appears at the back of this issue.