III. SOLID STATE PHYSICS

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A. THE QUANTUM MECHANICAL FOUNDATION OF THE THEORY OF SOLIDS

The separation of electronic and nuclear motions in the quantum mechanical treatment of molecules and crystals is based on the Born-Oppenheimer adiabatic approximation, according to which the electronic energy levels for fixed nuclei provide a potential for nuclear motion. In the case of degeneracy or near degeneracy of the electronic energy, the approximation may break down. We have started an investigation of the more detailed features of this method.

As a first step we have reconsidered the original paper of Born and Oppenheimer (1). In particular, we have examined the choice of expansion parameter $K = (m/M)^{1/4}$, motivating it physically and considering the effect of other choices of the order of the root.

A case of electronic energy degeneracy is provided by CO_2. This has been discussed in some detail by Renner (2). His method is being studied with a view to possible generalizations to other types of molecular symmetries.

T. D. Schultz

References

1. M. Born, R. Oppenheimer: Ann. Physik 84, 457, 1927
2. R. Renner: Z. Physik 92, 172, 1934

B. SOFT X-RAY VACUUM SPECTROGRAPH

We have obtained the M_{23} (valence to $3P_{3/2,\ 1/2}$) emission curves of copper and chromium. Both curves have sharp emission edges and clearly show the M_{23} separation.

In Fig. III-1 the experimental copper curve is plotted with the background eliminated and the ordinate divided by a factor proportional to the fourth power of the energy. The M_3 bands and M_2 bands are shown separated out by graphical means. The low-energy end of the curve is not reliable, and this part of the curve is emphasized by the E^4 factor. Therefore, the M_2 and M_3 bands were completed by the dotted lines at the low-energy end, showing the probable position of the bottom of the Brillouin zone.

In order to minimize the effect of fluctuations, the average of experimental chromium curves is plotted, modified by the E^4 factor in Fig. III-2. A representative curve is shown (dotted) for comparison. The M_2 bands and M_3 bands are completed by extrapolation. The results are summarized in Table I.

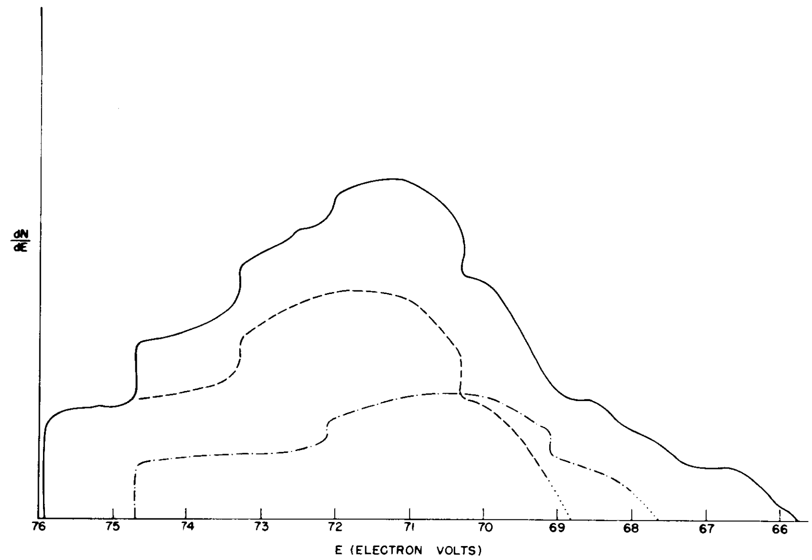

Fig. III-1.
Electron distribution in copper.

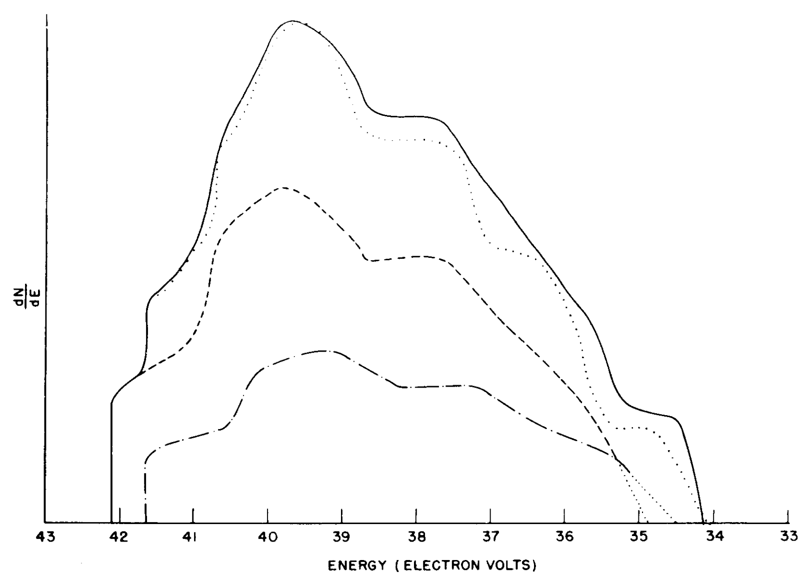

Fig. III-2.
Electron distribution in chromium.

Table I

Summary of Experimental Results

	Bandwidth (ev)	M_2 Emission Edge (ev)	M_{23} Separation (ev)	Ratio of M_3 to M_2 Intensities
Copper	7.1 ± 0.5	75.9 ± 0.2	1.2 ± 0.1	0.51 ± 0.03
Chromium	7.2 ± 1.0	42.1 ± 0.2	0.45 ± 0.1	0.52 ± 0.04

The results have been submitted to The Physical Review.

We have started the study of the nickel emission curve. We have been able to obtain sharp emission edges, but the remainder of the curve has not been reproducible. We are continuing work on this study.

The induction heater has been completed and during tests in a separate vacuum system it operated satisfactorily.

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C. MICROWAVE STUDY OF SEMICONDUCTORS

1. Electrical Properties of Germanium at Microwave Frequencies

Theoretical work on the solution of Maxwell's equations in a cylindrical cavity containing a semiconducting sample (1) has been completed by Dr. Hilda Hsieh. (It will be described in a technical report of the Solid State and Molecular Theory Group.) Dr. Hsieh's results predict that a transition of modes will occur when samples of different conductivity are placed in the cavity. For resistivities of the order of 15 ohm-cm, and greater, the resonator acts essentially as a perturbed cylindrical cavity; while for resistivities less than the order of 0.5 ohm-cm, the behavior is that of a coaxial cavity. A transition region occurs between these limits.

Bethe and Schwinger (2) used a perturbation approach to the problem which is satisfactory for small samples of low loss. Feenberg (3) obtained a solution for Maxwell's equations which is identical with Hsieh's first case, that of samples of such low loss that the imaginary component of frequency may be neglected. These methods are not applicable at all, in the strict sense, to germanium samples, but Hsieh's solution for the intermediate region shows that they may be used with fair accuracy up to values of $\tan \delta = 1$. For higher losses, however, Hsieh's solution alone is applicable, for the resonant frequency increases when the sample is inserted and, in the limit, approaches that of a coaxial cavity, as mentioned above.

Experiments have yielded results that are in agreement with these predictions. The high resistivity results have been mentioned previously (4). Measurements on an n-type sample of resistivity 0.6 ohm-cm yielded a value of 16 for the dielectric coefficient. Poor contact between sample and cavity was found to be the cause of anomalous results mentioned earlier (4).

Improvements are being made on the electronic equipment. As soon as they are completed, a series of measurements over a wide variety of samples will be made.

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References

1. H. H. T. Hsieh: Quarterly Progress Reports, Solid State and Molecular Theory Group, M.I.T. Jan. 15, 1952, April 15, 1952
2. H. A. Bethe, J. Schwinger: NDRC Report D1-117, 1943
3. E. Feenberg: Sperry Report GC 16907, New York, July 1942
4. J. M. Goldey: Quarterly Progress Report, Research Laboratory of Electronics, M.I.T. April 15, 1952