Extended and near edge structure of x-ray absorption spectra

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EXAFS *and Near Edge Structure* III. Eds. K. D. Hodgson, B. Hedman, and J. E. Penner-Hahn. Springer-Verlag, Berlin; Heidelberg; New York; Tokyo, 1984. pp. 533 (Springer Proceedings in Physics. V.2).

The book under review contains the materials of the III International conference devoted to a discussion of fundamental and applied problems associated with the fine structure of x-ray absorption spectra. The conference took place at Stanford University in the USA and attracted more than 200 participants. The transformation during the last decade of x-ray absorption spectroscopy into an independent field of scientific research was stimulated by the development in the middle 1970s of new methods of structural analysis based on the use of the so-acalled EXAFS spectra—the extended x-ray absorption fine structure. These methods that have acquired the common name of EXAFS-spectroscopy make it

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possible to study the close neighborhood of atoms of a given type in molecules, in crystalline and amorphous solids, and also on their surface. The unique nature of structural information which it is possible in a number of cases to obtain by analyzing EXAFS led to rapid development of EXAFS-spectroscopy and a growth of interest in the near edge structure of spectra—XANES (x-ray absorption near edge structure); the latter until now has not been widely used due to the complexity of interpretation.

The materials of the conference provide brief texts of 139 reports, grouped in 9 sections. The first section is devoted to the fundamental problems of the physics of x-ray absorption spectra. It includes 20 reports, in the majority of which problems of theoretical and experimental investigation of near edge structure—XANES are discussed. Different approaches to the theory of XANES are examined, and, in particular, it is shown that in some cases sensible results are obtained in utilizing approximations similar to those upon which the theory of EXAFS is based. The simultaneous publication of several papers describing the results of experimental investigation of the dependence of XANES on the direction of the polarization vector of the ionizing x-rays is noteworthy. Considerable attention in this first section is devoted also to the important, but so far insufficiently studied, question of the influence of many-electron effects on EXAFS and XANES-spectra.

The second section contains 7 reports, which examine the possibility of improving the methods of analyzing EXAFS-spectra in order to obtain from them structural data. The report of J. M. Tranquada proposes a method of determining the anharmonism parameters in crystals. D. V. Baxter discusses the method of determining the energy parameter E_0 in disordered systems which is important for interpreting EXAFS-spectra. Two more reports in the second section are also devoted to problems of EXAFS-spectroscopy of such systems. Sections 3–8 basically describe the results of specific structural investigations carried out by the methods of EXAFS-spectroscopy. In section 3,13 reports are presented which study the structure of the close neighborhood of heavy atoms in complex molecules of biological origin. The same section also includes 2 reports discussing the possibilities and the specific features of applying EXAFS-spectroscopy in investigating non-steady-state processes, and also the report by A. Bianconi which describes an effort to formulate recommendations useful for complex systems on determining special points in the XANES-spectra (ionization threshold, threshold of the continuous spectrum, etc.).

Section 4 which contains 16 reports is devoted to catalytically active systems and small metallic clusters. In a number of papers included in this section the methods of EXAFS-spectroscopy were used to study the close neighborhood of active centers which arise upon adsorption of atoms of transition elements on the surfaces of dielectrics. Other papers investigate the changes in interatomic distances in small metallic clusters compared with bulk systems, and also the structure of bimetallic clusters. In the interesting report by G. H. Yia, G. Meitzner, F. W. Lytle *et al.* which summarizes a large series of papers, it is shown that in bimetallic small clusters enrichment of their surface by one of the components always takes place.

In section 5 are collected papers that analyze the structure of the surface of solids by using EXAFS-spectra. (The methods intended for such purposes are called surface EXAFS or SEXAFS-spectroscopy.) The most interesting report in this section is the one by E. A. Stern, S. H. Heald, E. Keller *et al.*, where a new successful method of SEXAFS-spectroscopy is proposed based on the fact that the exciting radiation is directed to the surface of the sample at such a small angle that total external reflection occurs and predominantly the surface layer is excited.

Section 6 containing 19 reports is devoted to the investigation of amorphous materials and glasses. This field of application of EXAFS-spectroscopy is at the present time the most popular one. The section is preceded by two review papers by G. Bunker and C. E. Bouldin, and E. A. Stern and contains a description of the results of investigation of close order in a number of amorphous semiconducting and dielectric systems, and also metallic glasses. Section 7 brings together 13 papers describing results of studying minerals and solids at high pressures by using EXAFS-spectra. The most significant in this section appear to be the results of investigations of metamict phases and phase transitions at high pressure.

The fields of application of EXAFS-spectroscopy listed above are at present attracting the greatest attention, but they by no means exhaust all its possibilities. Section 8 of the conference materials contains 23 reports in which a broad selection of other structural problems are solved. The following items are examined: the structure of close neighborhood of atoms and molecules, imbedded in polymers; of ions in electrolytes; of impurity atoms in crystals; the processes of ordering in ionic conductors, the structure of intermetallic materials etc.

Section 9 contains 18 reports which investigate the fine structures observed in different spectra that are related in their origin to the fine structure of x-ray absorption spectra, and also the experimental technique in recording EXAFS and XANES. The reports discuss the fine structure observed in reflected x-ray spectra, in optical luminescence spectra excited by x rays, and in isochromats of bremsstrahlung spectra. New methods are examined of recording absorption spectra which make it possible to follow their change with time. The publication of two papers devoted to the development of laboratory EXAFS-spectrometers is noteworthy.

The book under review is of the greatest interest for specialists working in the field of x-ray and electron spectroscopy, but the circle of readers of whom this book may turn out to be useful and valuable is much broader. It includes the large number of physicists and chemists who are interested in new methods of structural investigations and their potentialities. Such readers without going into detail can obtain a sufficiently good idea concerning the principal problems that can be solved by the methods of EXAFS-spectroscopy and the prospects for its further development.