

Conference summary

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The series of XAFS Conferences has a tradition over about two decades. In the early days the main focus was towards a better understanding of the extended fine structure (EXAFS) itself. In the last decade the near edge structure attracted more attention again, e.g. since the York-conference (XAFS VI) the x-ray magnetic circular dichroism participated in this conference series with an increasing number of contributions. And we see in the present conference, that the spectacularly good energy resolution at 3rd generation machines attracts near edge spectroscopy again in performing chemical bond selective microscopy. We see that the measure of the x-ray absorption cross-section remains still the fundamental observable but with a changing focus. Also the quality of the x-ray beam has changed with time. At XAFS V to VIII (Seattle till Berlin) results of second generation machines were presented. The last 3 conferences from Grenoble (IX) to this Ako-conference (XI) have clearly benefited by the outcome of third generation synchrotron facilities.

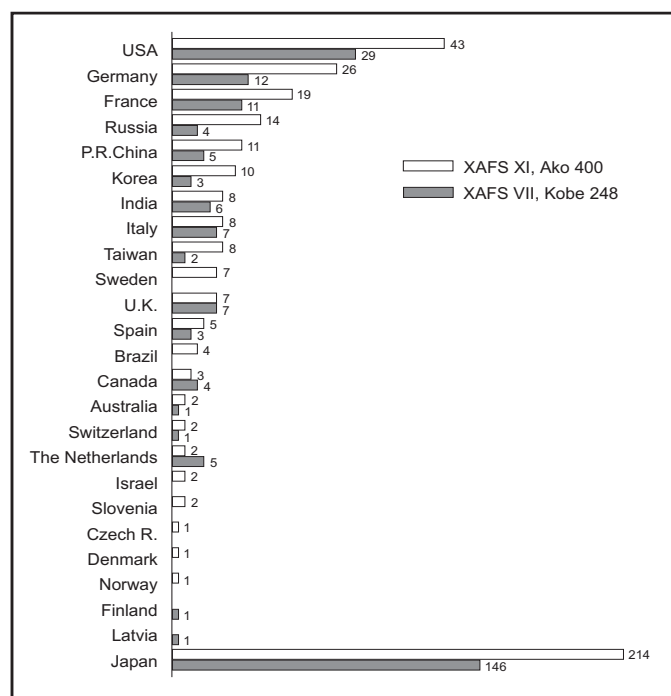


Figure 1

Number of participants listed per country for the Kobe- and Ako-conferences.

In the plenary lecture by D. Norman of prospects for super-bright light sources as well as in the “outstanding achievement award” lecture by E. A. Stern the view was turned to the future 4th generation facilities. It may appear that these super-bright sources (like XFEL) will address a different community; scanning of the photon energy to measure $\mu(E)$ may be less feasible, than one-shot experiments with samples mounted on a turbo pump blade.

Japan has hosted this conference series twice. In 1992 at XAFS VII in Kobe, the SPRING 8 facility started to be under construction. Today at the Ako-conference SPRING 8 is in full operation; at present it is the storage ring with the highest energy of 8 GeV, worldwide. The conference tour to visit SPRING 8 impressed all of the attendees, with its high (brilliant) performance and very broad range of user groups and fields. In Fig. 1 we list the number of participants per country. Most of the countries, be it the US, Europe or Asia, show an increasing number for XAFS XI (light bars). We also see new countries coming, like Slovenia, the Czech Rep., or Scandinavia. Not shown in the figure but very remarkable is the large number of contributions coming from Japanese industry. Already at the Kobe conference we saw a significant participation from the industry. To our observation the industrial research labs from Japan are worldwide the most active in contributing to XAFS-conferences. In Fig. 2 the contributions are listed by research topics. The “winners” are clearly catalysis and chemistry. The percentage of contributions in atomic and molecular physics is fairly small. An interesting and very positive feature of this conference series is the strong presence of theory. It happened for the first time at the XAFS VIII in Berlin that various theory groups came together and discussed the fundamental aspects of EXAFS among each other and with the experimentalists. That tradition is maintained over the years and we see it also here in Ako. During the last 5-6 conferences it became established to have three parallel sessions. The advantage is that a larger number of contributions do have oral presentations, the disadvantage is obvious a “normal” participant misses about 2/3 of the conference.

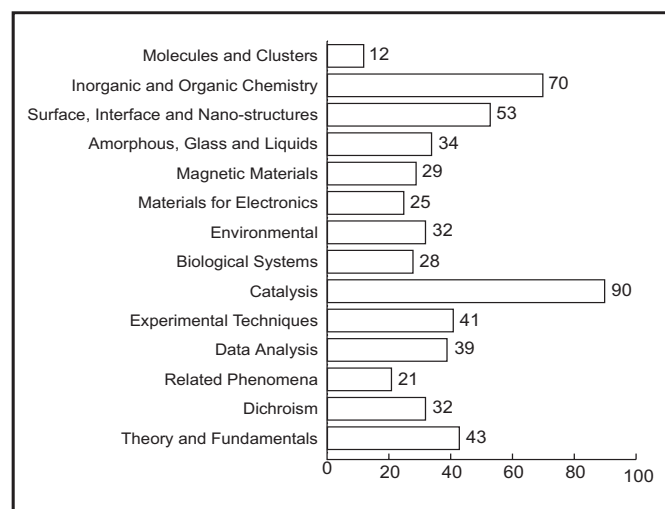


Figure 2

Number of contributions for different categories at the XAFS XI conference.

Below some of the highlights of XAFS XI are discussed: Time structure: in the first plenary talk (J. M. Thomas) Sir John presented time-resolved EXAFS for catalytic reactions. At the moment it takes still fractions of a second but in situ studies and detailed structural information on enzymes are very important and promising. Nice 3D-structure figures of enzymes were shown. A. Fontaine showed the design and operation of a micro coil at the ESRF which allows to study the dynamics of magnetic domain motions. By means of magnetic circular dichroism and the time structure of the bunches at the ESRF the response of magnetic domains

down to 20 ns was recorded. In the talk about future prospects by D. Norman the time structure of 50-100 femtoseconds/bunch for the fourth generation machines was discussed. Femtoseconds for a x-ray laser may allow pump-probe experiments addressing the characteristic time window for intra-atomic processes.

Energy resolution: the higher brightness and smaller emittance of synchrotron radiation leads to a better energy resolution particularly for monochromators in the soft x-ray regime i.e. the K-edges of C, N, O, etc. E. Rühl showed very high resolution in EXAFS-spectra (at BESSY II) in molecules like CO and NO which not only resolved the vibrational but also the rotational fine structure. Also high resolution spectra were taken at the ALS where the photosystem II was investigated. U. Bergmann could identify and separate the oxidation state of $Mn^{II,III,IV}$.

Also at the ALS impressive microscopy pictures of polymers were taken. A. Hitchcock showed pictures taken as monochromatic snapshots where the photon energy at the K-edge was stepwise tuned only by fractions of an eV, picking up the Carbon at different chemical environments. It seems that XAFS XI is the first conference showing the full applicability of soft x-ray spectromicroscopy for chemical industry. Microscopy of magnetic domains was shown using (i) photo-electron emission (A. Scholl), which is capable to see also antiferromagnetic domains, and (ii) a transmission x-ray microscope (P. Fischer) not depending on the surface sensitivity of PE.

Fig. 2 shows also that various investigations of material science were presented. H. Renever and coworkers investigated Fe_3O_4 with the well known metal-insulator transition and asked the question for the Fe^{3+} - Fe^{4+} charge ordering. Can x-ray-scattering detect charge ordering? Their results show no separate shifts of the Fe-edges corresponding to 3+ and 4+ ionicity. All Fe ions seem to have the same ionicity of 2.5+; no charge ordering! In another example Surface EXAFS was used to study the epitaxial growth of ultrathin Ni/Co films. These pseudomorphic grown structures are new artificial materials. Diffraction techniques using x-rays or low energy electrons give structural information averaged over a larger area. D. Chanderis (LURE) showed how powerful EXAFS can be to distinguish from a local point of view bcc versus fcc structures. XAFS is an important tool to determine the chemical state of a specific element. This was applied in environmental science by D. Sayers to study the contamination of soils. A new polarization-dependent XAFS instrument under total reflection and in the fluorescence mode was presented by K. Asakura to study catalytic reactions on single crystal surfaces.

Further progress in the application of dichroism was presented. H. Maruyama used a helicity modulation method to study XMCD between 6 – 16 keV at SPRING 8 improving S/N ratio and efficiency. D. Arvanitis demonstrated that the degree of transverse coherence of the synchrotron beam (at 5 different facilities) has influence on the white line intensity and XMCD analysis. H. Wende showed temperature dependent MSRD in the magnetic EXAFS giving access to a "spin-pair distribution" function.

A better analysis and understanding of x-ray absorption spectroscopy was demonstrated at many cases in this conference, we

name only few. L. Tröger showed experiments taken at HASY-LAB in which one does not only see the commonly discussed interference pattern of the photoelectron wave but also the photon interference of the x-rays in the EXAFS fine structure (PIX-AFS). A. Kodre discussed the atomic (oscillatory) background in the extended x-ray spectra for gaseous hydrides of Ge, As etc. This Atomic XAFS was discussed in the Chicago conference for liquid catalysts and solids before. Further progress was made in the analysis of higher order contributions in the amplitude and phase of EXAFS. T. Yokoyama used the path integral approach to calculate the temperature dependent mean square relative displacement as well as the anharmonic vibrations in solids.

It was said in the beginning that at EXAFS conferences also many active and powerful theory groups come together and form an important basis for better understanding of the x-ray absorption spectroscopy. One might say that at the Ako-conference we also see a third generation theory (J. J. Rehr in his plenary talk). In early years each set of data was fitted by theoretical means with an individual set of parameters. Today almost no adjustable parameters are left over - all experimentally "free variables" are implemented in the theory. For the real space multiple scattering approach (e.g. FEFF) this is the temperature dependence, the angular dependence and very recently the spin dependence. Nowadays the user has the option to use an expansion in higher order scattering paths or alternatively a full matrix inversion. Also the real and imaginary parts of the scattering amplitude f' and f'' are implemented which is very important for DAfS (J. Cross). Another excellent example for a symbiosis between theory and experiment is the development of natural dichroism. C. R. Natoli discussed the theory of this dichroism in chiral structures using the framework of multiple scattering and circular dichroism. This field is an excellent example in which the helicity of the synchrotron radiation must be changed from left hand to right hand since no magnetization is present and no switching of external magnetic fields from plus to minus can be used. Theoretical progress was made in many aspects, e.g. A. Kotani gave an overview on resonant x-ray emission spectroscopy including the polarization dependence. T. Fujikawa discussed many body effects in XAFS.

Last not least let us mention the two Young Scientist Awardees. A. Filipponi used XAFS to study supercooling in liquid metals and A. Ankudinov presented a theory which connects the XAS to the projected atomic density of states. With this technique one overcomes difficulties in XMCD analysis and hole counting in the final d-states.

In summary XAFS XI, the Ako-conference, shows advances on the level of third generation everywhere, be it the performance of the synchrotron radiation (SPRING 8), and the unified theory. All of us enjoyed the great hospitality at the historical site of the 47 loyal Samurai. The next conference XAFS XII will be held in summer 2003 in southern Sweden, Lund, at the site of MAXLAB. For further information see <http://www.XAFSXI.MAXLAB.lu.se/>. Also XAFS XIII has been decided to take place at the Stanford Synchrotron Radiation Laboratory in 2006.