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CAMOP: Report on the 20th International Conference on X-ray and Inner-Shell Processes, 4–8 July 2005, Melbourne, Australia

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Abstract
The 20th International Conference on X-ray and Inner-Shell Processes, X05, was held at the University of Melbourne, VI, Australia, on 4–8 July 2005. A selection of the papers presented at this meeting is briefly summarized and commented upon. Diverse areas of atomic and condensed matter physics in theory and experiment are undergoing vigorous and stimulating development with a variety of novel applications.

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1. The conference

The 20th International Conference on X-ray and Inner-Shell Processes, X05, was held at the University of Melbourne, VI, Australia, on 4–8 July 2005. This was the latest meeting in the long-standing conference series 'X-ray and Inner-Shell Processes' dedicated to x-ray science and atomic and condensed matter theory and application. The current series is a unification of the earlier separate series of 'Conferences on X-rays' started in 1965 (held both in Ithaca and Leipzig) and continued until 1976 (Washington), and the series on 'Inner-Shell Ionization' (held in 1972 in Atlanta and 1976 in Freiburg). The meetings in the joint series were held in Sendai, Japan (1978), Stirling, Scotland (1980), Leipzig, Germany (1984), Paris, France (1987), Knoxville, USA (1990), Eugene, USA (1992), Debrecen, Hungary (1993), Hamburg, Germany (1996), Chicago, USA (1999) and Rome, Italy (2002).

The nature of the conference has evolved over time, and the brightness and incisiveness of synchrotron facilities now play a major role in many of the plenary, invited and contributed presentations. However, accelerators, storage rings, fixed x-ray sources and novel sources such as electron beam ion traps play continuing and new roles in the development of the field. Additionally, some presentations relate to yet other sources, and in particular soft x-ray generation from high-power, high-brightness lasers and indeed the most powerful laser sources in the world. Other presentations relate more to an increased understanding of the processes involved in inner shells or solid state interactions than to areas of conventional x-ray energies alone. Indeed, some detail the use of electrons or infrared radiation to elucidate structure and provide new insights.

Delegates have registered from over 27 countries and all around Australia. The fundamental research drives exciting developments in synchrotron techniques. It underpins innovations in applied science from medicine to nanotechnology that benefit communities and industry. X05 has been an excellent opportunity to share insights with leaders in key emerging and developed fields.

Subjects that were once regarded as purely fundamental research in experimental and theoretical atomic and molecular physics now make vital contributions in these proceedings to the development of new materials, forensic sciences, pharmaceuticals and metrology standards. Emerging fields include the generation of intense x-ray sources, imaging techniques, and the design of instrumentation and synchrotron beamlines, as well as the detailed understanding that access to synchrotron light sources affords us in our efforts to elucidate the nature of fundamental electronic processes.

We received 250 abstracts and over 180 participants. The programme included 5 plenaries, 20 invited oral presentations, 56 other oral presentations, and 156 presentations in two

strong poster sessions. A number of sessions were conducted in parallel. The invited speakers, chosen from among many suggested by the members of the International Scientific Committee and the Advisory Committee, reviewed the latest developments in the fields. The X05 proceedings will soon be published in a special edition of Radiation Physics and Chemistry [1].

2. Atomic physics of photoionization: developments and challenges

The conference opened with a distinguished plenary and overview of atomic interactions with (x-ray) radiation by R H Pratt (Pittsburgh). Much development of theory over the past decades was reviewed, to the current very high state of maturity of the field [2]. In a variety of experimental regimes, but particularly in the angular dependence of elastic and inelastic scattering and for both bound–free and free–free (bremsstrahlung) processes, it was well argued that higher multipoles can (and often do) play a significant and observable role in recent experiments. Extension is being made to the (multiple) photoionization of molecules and clusters, and to inverse processes including radiative electron capture.

Despite this excellent overall understanding and the success of atomic theory, there are major discrepancies between existing theoretical and experimental tabulations and formalisms. Discrepancies between different theoretical computations are due in part to different treatment of relativistic effects, convergence issues, the inclusion or otherwise of higher multipole interactions, and possible general limitations of validity of specific approaches [3, 4].

Another major outcome of this conference was the general realization that experiments can now obtain results up to ten times more accurately (or possibly much more) than theoretical treatments. This is a major challenge to theory in general, and permits both criticism and provides insight to a wide range of modelling assumptions and approaches. There was a key question in this discussion which focused on the acknowledgment of this experimental accuracy, but asked 'In what range of energy and for what range of atomic number do these new (solid state) experimental results inform the atomic, gas phase or isolated atom investigations of absorption, scattering, and (atomic) electronic wavefunctions?'

A partial answer has been provided [5] supported by the observation and theoretical predictions that far from the near-edge fine structure, the experimental results should correspond well with an atomic ideal down to any detectable level. In the near-edge regime (e.g. within 1–3% of the edge energy), there appear to be key features which remain atomic in nature and are not well (or reproducibly) computed in most current formalisms, so that the prospect in this regime is somewhat different. This new challenge will be taken up by theorists, and may be summarized as: 'How can a computation of neutral-atom inner-shell behaviour for $Z > 3$ be made in any regime to an accuracy of 0.03%, or even to an accuracy better than 1%?' Of course we do not include hydrogen or helium themselves in this question, as the relevant accuracy for particular transitions in this regard was surpassed long ago.

An insight to the first question has been provided by the presentation of A Kodre (Ljubljana, Slovenia) on the x-ray absorption of monoatomic (gaseous and non-diatomic) iodine. Previous work has addressed atomic vapours directly [6]. In a careful and meticulous experiment from 300 °C to 1000 °C, the dissociation of the molecular binding is shown to progressively shift the photoexcitation spectrum in the x-ray absorption near-edge structure (XANES). Hence the limit of fully dissociated iodine is then an indication of the atomic, isolated atom spectrum.

Another part of this question has been addressed by the presentation of U Hergenhahn (Tohoku, Japan) by investigating near-edge shake processes (e.g. resonance processes involving an intermediate doubly excited state) in atomic neon. The structures observed there confirm post-collision interaction theory and the atomic nature of this structure. These developments have some impact upon the controversy relating to 'atomic XAFS' (x-ray absorption fine structure) in the sense that isolated atoms can certainly have near-edge structure. This also impacts upon the approaches to near-edge structure in solid state physics, below, which conventionally assume that the 'atomic base-line' is smooth and structure free.

In the area of dipole and non-dipole interactions in photoelectron angular distributions, there were several interesting presentations surrounding a current controversy. R H Pratt correctly noted that in a variety of experiments non-dipole processes are essential, and that angular distributions of scattered photons or of photoelectrons would be ideal examples of such a situation. Reports by S H Southworth (Argonne, USA) and others supported this; but another presentation (A Yagishita, Photon Factory, KEK, Japan) found no such dependence in a similar experiment on molecular nitrogen, in contrast to the earlier work of Hemmers *et al* [7]. This is currently a mystery, although there are really two classes of experimental apparatus involved, and this reviewer believes that one class of experiment may average over orientations in some manner, while the other may see the 'expected' non-dipole asymmetries. I look forward to further developments in this field.

Double K-shell photoionization was addressed in several presentations, including those of E Kanter (Argonne, USA) and J-Cl Dousse (Fribourg, Switzerland). The dependence of this process upon Z has been revisited recently, and it now appears important to separate the dependencies of shake-off processes (loosely, intermediate excited states followed by ionization) from a dynamic electron–electron scattering term. It is now possible to compare photoionization hypersatellite spectra of solid targets (e.g. of Mg) with the accelerator-induced hypersatellite spectra obtained some time ago [8].

3. Atomic physics of inner-shell transitions: theory and experiment

M Deutsch (Bar-Ilan, Israel) presented an outstanding plenary full of new results in the characterization of characteristic lines and synchrotron photoabsorption and fluorescence of these photons in a two-stage process. His earlier work on high-resolution, high-accuracy determination of Kα and Kβ spectral lines is well known, and has defined several of the

key wavelength standards in the x-ray regime. A worrying problem for experimentalists attempting to make high-accuracy measurements was the questionable profile stability of conventional electron-impact characteristic spectra, as a function of impurities or accelerating voltage. A common rule of thumb has been to ensure that the accelerating voltage is at least two or three times the energy of the spectrum of interest.

In past work, the group of Deutsch has characterized the satellite spectra of several key characteristic lines. In this presentation, he has shown that a synchrotron photon excitation or ionization at threshold, near the edge and far from threshold reveals the development of this satellite spectrum in a clear manner. The high-resolution, structural evolution with energy constitutes a breakthrough, and serves as a partial quantification of the sorts of effects that past researchers using characteristic sources would worry about without being able to quantify them.

Numerous other papers were presented in this field, with some interesting results. N A Borovoy (Kiev, Ukraine) also presented work near-and-far from threshhold; J Hoszowska (ESRF, France) demonstrated the particulate size dependence of the characteristic spectra; K Ilakovac (Zagreb, Croatia) investigated the two-photon decay of K-shell vacancies. Numerous other poster presentations contributed usefully to this subject.

4. Condensed matter physics of photoionization: new opportunities

Turning to the solid state aspects of structure, and the diagnosis of local environments by XAFS measurements and related techniques, J J Rehr gave an excellent review of XAFS and an overview of his group's recent efforts which are widely used and acknowledged throughout the world. The determination of bond lengths, Debye temperature parameters and related local structural information has led to thousands of papers in the literature, and is one of the three most common applications of synchrotron research.

Rehr stated the goal (or dream, or revolution), which several of us are hoping for in the not-too-distant future, that XAFS analysis will become a direct *ab initio* technique for structure determination complementary to crystallography while also able to target local or disordered systems, including alloys, interfaces and solutions. He also discussed key opportunities for the future in the area of improved modelling of thermal and disorder parameters, intrinsic losses of the photo-electron amplitudes, and the possible contributions of Bayesian statistics and a real-space Green's function approach to the problem. The plenary also broadened the discussion to discuss the utility of the formalism to investigations of x-ray emission spectroscopy, non-resonant inelastic x-ray spectroscopy and related experiments.

In one sense, there was a confident feeling of success from past accomplishments, as was evinced by the many presentations at the conference using the standard analysis developed by Rehr. In another sense, there were several key fundamental issues to be addressed in the near future, which involved many discussions over lunch and elsewhere between attendees.

In particular, the presentation of A V Soldatov (Rostov State University, Russia) was based on the experimental and theoretical framework for investigating clusters, as a natural bridge between isolated atoms and solids with macroscopic dimensions. In this regime, the muffin-tin potentials of Rehr may actually work well, on the average, but in numerous regimes will be expected to fail, and a non-muffin-tin approach will become essential. Any variation with cluster size is not well represented by muffin-tin or Full Linear Augmented Plane Wave (FLAPW) approaches [9], which more generally represent 'infinite' mathematical solids; and any local asymmetry is also best represented with a non-muffin-tin potential. In the literature, several authors have argued that this may be true, but that the muffin-tin approaches are 'succeeding in all applications', so there is 'no need' to investigate further. Of course, this often depends upon how critical the data is for the application in question.

Soldatov presented interesting data on cluster-deposition, assessing the size of clusters, and then simulations of the near-edge structure using a synthesis of FDMNES (finite difference method for near-edge structure) code. These examples required non-muffin-tin approaches for their elucidation.

Some key successes were outlined in this talk and in other presentations, including those of C Witte (Melbourne, Australia) who showed strengths and limitations of current FDMNES code, and proving that the FDM code can be extended (with some effort!) well beyond the near-edge regime; and L F Smale (Melbourne, Australia) who showed strengths and limitations of the latest muffin-tin code when applied to high-quality data [5, 10]. This work demonstrated the difficulty of achieving appropriate error analysis with conventional analysis, and explored solutions to this problem. The presentation observed that it is experimentally possible to obtain data from a symmetric and infinite solid which therefore should be able to be modelled by muffin-tin approaches except for the treatment of boundaries and discontinuities. It is then possible to achieve fits which appear to be 'very good' by visual inspection using this muffin-tin approach; and yet the minimum accurate χ_r^2 values of over 100 even with a narrow fitting window indicate limitations of the existing approaches. This strongly argues for the need for improved models and for the need to treat even 'extended XAFS' as still lying in the 'near-edge regime'. Exciting future work will address these unresolved problems and opportunities.

5. Scattering of atomic and condensed matter

The processes of inelastic and elastic scattering received no less attention in the conference. T Suric (Zagreb, Croatia) presented a development of the impulse approximation to include dynamic effects, correlations and non-local exchange corrections for doubly differential cross-sections (as a function of outgoing photon energy and angle). This then goes beyond the IPA (independent particle approximation) and shows promise in the determination and interpretation of Compton scattering.

M J Cooper (Warwick, UK) presented latest results of a Compton scattering study of 4f ferromagnetism (in fact,

of spin density) using high-energy elliptically polarized synchrotron radiation. This study serves to categorise particular complex and controversial ferromagnets in terms of their characteristic orbital type. The talk was much broader than this and also reviewed the field of magnetic Compton scattering, the subject of a recent text [11].

A detailed theoretical and experimental comparison of resonant inelastic x-ray scattering (RIXS) was presented by A Kotani (RIKEN, Japan) with particular application to recent data on NiO. A Bosak (ESRF, France) probed the phonon density of states from inelastic x-ray scattering, and investigated the ability of theoretical models to determine Debye temperatures and the vibrational density of states. D A Bradley (Exeter, UK) investigated elastic scattering from dilute solutions in the near-edge regime, particularly in order to assess the utility of the IPA in this regime. In turn, this allows a comparison with form factors and anomalous (absorption) fine structure for scattering. Numerous other presentations also contributed to these fields.

6. Investigations of few-electron systems and tests of QED

As is conventional in this series of conferences, the focus of investigation is not restricted to neutral species or low-ionization states. In fact, many of the 'best' tests of fundamental aspects of theory and computational frameworks are still provided by 'simple' few-electron systems, and in particular these can provide critical tests of quantum electrodynamics (QED) which underlies all the theoretical work at the conference (and indeed in atomic and condensed matter physics).

P H Mokler (GSI, Darmstadt, Germany) gave an excellent overview of great progress made over the recent decades on the Lamb shift in heavy atomic systems. Dielectronic recombination and other processes and accelerator (storage ring) experiments were reviewed and discussed, and the great achievements of GSI, LBL and other major accelerators were highlighted. In particular, investigations of helium-like and lithium-like systems have provided critical insight into higher-order processes and two-electron QED.

P Beiersdorfer (Lawrence Livermore National Laboratory, USA) has provided many of the results in the literature for relative calibration of spectral lines in the few-electron systems, by using discharge sources or electron-beam ion traps (EBITs). Following this work, he presented a new survey of polarizations of a series of lithium-like, helium-like and hydrogenic resonance x-ray spectra. The relative polarizations are a sensitive indicator of the production process of the highly charged ions in the EBIT (or other source) and a test of the implementation of atomic physics in this environment. Hence this polarization data clarify the assumptions made regarding satellites and transition rates.

J R Crespo Lopez-Urrutia (MPI Kernphysik, Germany) presented the first results from the new Heidelberg EBIT, and investigated state-selective quantum interference in the radiative and dielectronic recombination channels in mercury around resonance transitions.

G W F Drake (Windsor, ON, Canada) focused on recent key advances in atomic theory for relativistic and QED effects in (low-Z) atomic helium and lithium, and in applications of this theory and corresponding experiments to nuclear physics and in particular to the nuclear charge radii of isotopes. M N Kinnane (Melbourne, Australia) in turn reviewed recent experimental advances and the development of tools and techniques in the measurement of QED in the medium-Z regime. Future results in these areas will be of great interest.

7. New laser plasma x-ray sources and studies towards higher brightness and flux

Two of the plenaries of the conference addressed exciting new sources and their potential applications. M Murnane (JILA, Boulder, USA) gave an overview of her group's outstanding developments in nonlinear optics towards viable VUV lasers and higher harmonic spectra corresponding to x-ray beams with significant coherence properties and flux. She discussed attosecond laser pulses and applications, and particularly addressed the challenges to produce a clean, high-flux bright coherent beam in the x-ray regime. The technical requirements of this challenge are formidable, but progress has been very promising and encouraging. Effectively this does not replace the goals for a free-electron laser but instead serves as a complementary regime with numerous interesting and useful applications.

The last plenary, L T Hudson (NIST, Gaithersburg, USA), went to even higher power and flux, and discussed x-ray spectroscopy at next-generation Inertial Confinement Fusion (ICF) sources. In particular the OMEGA and NIF laser sources have produced recognizable few-electron x-ray spectra, and the challenges to even observe this with an x-ray diagnostic or spectrometer are immense. The 60-beam OMEGA system, at the University or Rochester, is a 30 kJ, ultraviolet (351 nm), pulse-shaped, direct-drive laser with on-target irradiation nonuniformities approaching the 1–2% level. The upcoming National Ignition Facility (NIF) is even larger and more powerful. How can you build a scientific precision instrument to deal with a very large electro-magnetic pulse event and not even lose resolution? And how can a spectrometer collect data in this environment in the presence of very large particulate scatter and potentially overwhelming background fluorescence? Hudson enumerated many of the challenges (and some of the solutions) to his group's successful observations and clean, moderate-precision results. Another talk by C Szabo from Hudson's group also addressed the challenges of fluorescent background using convex-crystal spectrometers. One of the key problems for the future is the extension to even higher fluxes, to free-electron lasers, and to a quantitative interpretation of the results.

Some of these questions above have been addressed this year in difficult laser-synchrotron pump-probe experiments by Argonne, and presented by L Young (Argonne, IL, USA). This was the first presentation of some of the overview, and was a clear and outstanding result of experimental science and of interpretation.

I A Ivanov (ANU, Australia) discussed multi-photon lasers and higher harmonic production within a theoretical framework. Several other presentations addressed this growing and developing series of opportunities and dilemmas in the high-coherence, high-brightness regime that many are hoping will be realized with free-electron lasers.

8. Novel and critical applications of technology and insights for biomedicine, chemistry and earth science

Interesting and important applications of the technology of the earlier areas were presented in numerous talks and many posters. A pleasing feature of these submissions was that an increasing fraction of the presentations on XAFS or XANES for example were critical applications requiring good or high quality data in order to elucidate new structure and insight. This reporter presented an overview of a critical new technique for collecting high-accuracy XAFS data (the x-ray extended range technique, XERT).

S P Best (Melbourne, Australia) showed that EXAFS was sensitive to and could determine or confirm the relevant unstable reduction products of intermediates in hydrogenase cluster catalysis.

G Lucovsky (UC Santa Barbara, USA) showed how nano-crystallinity by Jahn–Teller term splittings in XAFS could be a much more sensitive and insightful probe for small-scale crystallinity than other conventional probes (if the appropriate data sets are collected and analysed carefully).

A Marcelli (INFN, Italy) discussed how polarized XANES can identify local distortions in the two orthogonal directions, usually parallel and perpendicular to structural or lattice planes in the sample or anisotropic cluster. Use of clean polarization-sensitive experiments of this type is at an early stage, but this approach gives extra insight and handles into the resolution and characterization of samples.

Strong presentations from the group of Z Wu (Beijing SRF, China) emphasized biological applications of XAFS to metalloproteins, and described beam lines being constructed for that purpose.

Structural investigations of lattice defects in quantum dot formation were also analysed by researchers from Russia (S Nikitenko, Novosibirsk) and strong presentations on many other areas were given.

The shake processes are very significant in near-edge photoelectron spectroscopy, and this was the subject of several presentations including those of B Brena (RIT, Stockholm, Sweden) and U Hergenhahn (Tohoku, Japan).

T Koide (Photon Factory, Tsukuba, Japan) presented applications of angle-resolved soft x-ray magnetic circular dichroism to Fe/MgO/Fe tunnel magnetoresistance.

M Vos (ANU, Australia) described the successful application of (e, 2e) electron momentum spectroscopy to probe electron orbital wavefunctions in atoms and molecules and in particular, application to heavy systems including gold thin films.

Several presentations were made on fragmentation and electron–ion coincidence studies of ultrafast dissociation of molecules and of Auger processes, including those of K Ito (Tsukuba, Japan), K C Prince (Sincrotrone Trieste, Italy) and G Pruemper (Tohoku, Japan).

9. New detectors, spectrometers and instrumentation

E N Ragozin (P N Lebedev Physics Institute, Moscow, Russia) discussed the design of aperiodic multilayer mirrors and their application. E Sato (Iwate Medical University, Japan) explained applications to phase-contrast radiography and enhanced K-edge angiography with a local source compared to a synchrotron environment. T Hatsui (Okazaki, Japan) descibed a transmission grating spectrometer for soft x-ray studies. J Luning (SSRL, USA) highlighted some key opportunities in x-ray Fourier transform holography for imaging nano-scale samples. R Leckey (La Trobe, Australia) described a new toroidal analyser used to obtain photoelectron diffraction data to determine atom positions on surfaces and in bulk, and interpreted results for corresponding Kikuchi lines in terms of single-scattering processes. Several presentations addressed new imaging, tomography and related techniques.

10. Hot topics and summary

The conference had two ‘hot topics’ Sessions. Amongst these selected talks, N Berrah (Western Michigan University, USA) described work on Feshbach resonances in negative ions, and double Auger decay, and some of the latest results in this difficult experimental regime. U Becker (Fritz–Haber-Institut der MPG, Berlin) discussed the transition between non-localization and localization in molecular nitrogen, which can be observed by isotope-substituted K-shell photoemission. Numerous other talks and posters were worthy of mention, but this is a representative summary of at least a significant part of the excitement of this conference and the fields involved.

With the strong thread of new exciting insights, technology, applications and science running through these presentations, it is clear that this series of conferences, and the fields that it represents, has a very strong and vigorous future.

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