

CCP3

SURFACE

SCIENCE

NEWSLETTER

Collaborative Computational Project 3
on Surface Science

Number 29 - July 2001

ISSN 1367-370X



Daresbury Laboratory



Contents

1	Editorial	1
2	News from the Project	3
2.1	Flagship Grant	3
2.2	e-Science	3
2.3	Training Workshop	3
3	Update on CCP3 Projects	4
3.1	DL Visualize News	4
4	CRYSTAL-2001	6
5	Lab Reports	7
5.1	Richard Lambert, Department of Chemistry, University of Cambridge	7
5.1.1	STUDIES ON TiO ₂ AND TiO ₂ /METAL SYSTEMS.	7
5.1.2	EPOXIDATION OF STYRENE ON Cu(111) AND (110)	8
5.1.3	ALKENE EPOXIDATION ON SILVER SURFACES AND THE EFFECTS OF OXY-ANION PROMOTERS	8
5.1.4	AFM STUDIES OF THE GENESIS OF SILVER ON ALPHA ALLUMINA ETHELENE EPOXIDATION CATALYST	9
5.1.5	ELECTROCHEMICAL PROMOTION OF THIN FILM METAL CATALYSTS	9
5.1.6	OXIDATIVE COUPLING OF METHANE (OCM)	10
5.2	Surface structure and electronic structure: Phil Woodruff, Depart- ment of Physics, University of Warwick	11
6	Programming Tools	15
6.1	Version Management Systems for Code Development: An Introduc- tion to CVS	15
6.2	Shared Memory Parallelism with OpenMP	17
6.3	Java for Scientific Computing	19
6.3.1	Getting Started	19

6.3.2	About Java	20
6.3.3	Programming tools for Java Developers	22
6.3.4	Useful Java libraries	22
6.4	Fortran95 for Fortran77 Programers	23
7	Training Day	27
8	News from the Synchrotron Radiation Research Theory Network: SRRTNet	29
9	Links	30
10	Meetings	32
10.1	Calendar of Meetings and Workshops	32
11	Members of the working group	34

Contributions to the newsletter from all CCP3 members are welcome and should be sent to ccp3@dl.ac.uk.

Editor: Dr Adrian Wander

Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK

1 Editorial

It has been a mixed few months for CCP3. Most obviously, we have suffered two major disappointments in respect of EPSRC funding; they are detailed elsewhere in this newsletter. First, in April, we heard that our proposal for continuation of CCP3's funding, and for an associated flagship project on the simulation of surface-deposited metal nanoparticles to be based at Imperial College, had been turned down. This presents us with an immediate problem; at the steering group meeting held in April, just after this result became known, it was decided to submit as quickly as possible an alternative flagship project, based on a much-needed development of the EXCURV software for the analysis of EXAFS data. This flagship project represents a renewed emphasis on the instrument support side of our activities, and we think it represents an exceptionally strong case in terms of its overall benefit to the surface science community. We shall see whether the EPSRC panel agrees with us!

Our second disappointment involved a new EPSRC initiative—that in GRID computing. Many of you will have seen the publicity surrounding the allocation to EPSRC of substantial funding for the development of 'e-science', and its subsequent decision to invest in a number of large-scale 'testbed' projects for the development of scientific applications of grid computing. Under the leadership of Mike Allen, who chairs the steering group made up of all the CCPs, we put in a bid on behalf of all the CCPs stressing the diverse uses that the various CCP communities could make of the new possibilities opened up by the GRID. Unfortunately, although we were among those shortlisted and invited to submit a full proposal, we were unsuccessful at the final stage.

These disappointments were all the more intense because a great deal of work had been put into the proposals. I would like to take this opportunity to thank on behalf of CCP3 those involved (both in those proposals that were, sadly, unsuccessful and in the one currently under consideration); in particular Nic Harrison, Adrian Wander, John Inglesfield, Paul Durham, Mike Allen and John Harding (chair of CCP5, who coordinated the section within the GRID proposal on multiscale simulation, within which most of the CCP3 interest lay).

We are not alone in our disappointment; some of you will have seen the email from Mike Allen that I circulated to the CCP3 working group at his request, expressing his disquiet at the selection process for the GRID proposals. It is also clear from comments at the CCP steering group that many CCPs are currently having trouble with getting renewal proposals through the EPSRC peer review process.

But I said it had been a mixed period—what of the good news? There is plenty, much of it described in this issue. SRRTnet, the international synchrotron theory network that is largely modelled on CCP3, is making a strong start and we will be hosting the first code training day sponsored by its European arm this autumn. The codes from

previous CCP3 flagship projects continue to develop for the benefit of the surface science community. The scientific vibrancy of our member groups is clear from the two lab reports in this issue. And our Daresbury team have started a series of articles designed to introduce new computing tools to the scientific community. Looking ahead, both the new synchrotron and the free-electron laser facility planned for the Daresbury site will provide new opportunities for surface science, and substantial new challenges for analysis—challenges that it will be CCP3’s job to meet.

I would like to finish by one more thank you—to John Inglesfield, who stepped down as Chair of CCP3 at the beginning of the year. Happily he will continue to be closely involved with us, and is one of the Co-Investigators on the new renewal proposal. The healthy state of CCP3 and of its program library is a great tribute to his stewardship, and has made my life a lot easier!

Andrew Fisher, UCL.

2 News from the Project

2.1 Flagship Grant

The CCP3 flagship grant for the development of new methodologies for the study of metal clusters on oxide surfaces was unsuccessful. The grant will be resubmitted in the Autumn. A new flagship grant for the development of techniques for the analysis of EXAFS/XANES spectra has been prepared in collaboration with the X-ray Spectroscopy Group of the Synchrotron Radiation Department at Daresbury. This was submitted in June. Hopefully we will have news of this grant in time for the next issue of the newsletter.

2.2 e-Science

CCP3 was also closely involved with a cross CCP proposal which aimed to produce a grid test-bed application. CCP3 proposed a project aimed at the direct simulation of nano-scale systems including parts that are physically well separated and/or weakly coupled. Different levels of theory (atomistic, continuum, statistical) could be used for various parts. An example of such a system would be a self-assembled pattern of nanoparticles on a metal surface coupled by a strain field. The project aimed to produce methods of specifying the partitioning of the system; taking in to account both the varying bandwidth requirements between components and the amounts of computer power required for each component. Some communication of information (such as boundary conditions) between components would be necessary, but this information is a small fraction of the total datasets needed to describe the system. If two components become strongly coupled; the calculation could be reconfigured so that they run on the same computer or on machines closely coupled by a fast local network. This grant request was also unsuccessful and we are currently exploring ways of taking this exciting project forward.

2.3 Training Workshop

CCP3 and SRRTNet are planning a code training workshop for November 2001. The workshop will introduce new users to the suite of programs developed by the projects. Attendance at the workshop is free, but places are limited: see section 6 for details of how to register.

3 Update on CCP3 Projects

3.1 DL Visualize News

DL Visualize version 2.1 is now available. This version features an interface to the CRYSTAL98 software package. The new version provides the ability to construct and visualize crystals, surfaces and molecules. The graphical user interface to CRYSTAL98 provides a simply and intuitive method of setting up input decks, and provides a powerful method of analysing the wavefunctions generated by CRYSTAL98 and hence of calculating associated properties. The code also provides a simple method of generating LEED patterns from complex surfaces and can provide both single domain and multiple domain patterns.

The new release is available for Compaq Tru64, SGI Irix 6.5, Sun Solaris 8, IBM AIX 4.3, Windows and Linux (RedHat 6, SuSe 7) and will provide the following functionality:

- calculation and display of LEED patterns.
- identification of the Miller indices of crystal and slab directions.
- saving displayed structures as images or VRML.
- support for 2D and 3D datasets.
- an interface to CRYSTAL98.

The CRYSTAL98 interface has support for

- running SCF jobs locally or remotely.
- displaying charge and spin density isosurfaces or contour maps.
- density of states plots.
- band structure plots.

The upgrade is free to current DLV users. New users can register for free demo licences via the [DLV web site](#) where more information is available.

Barry Searle, CLRC Daresbury Laboratory

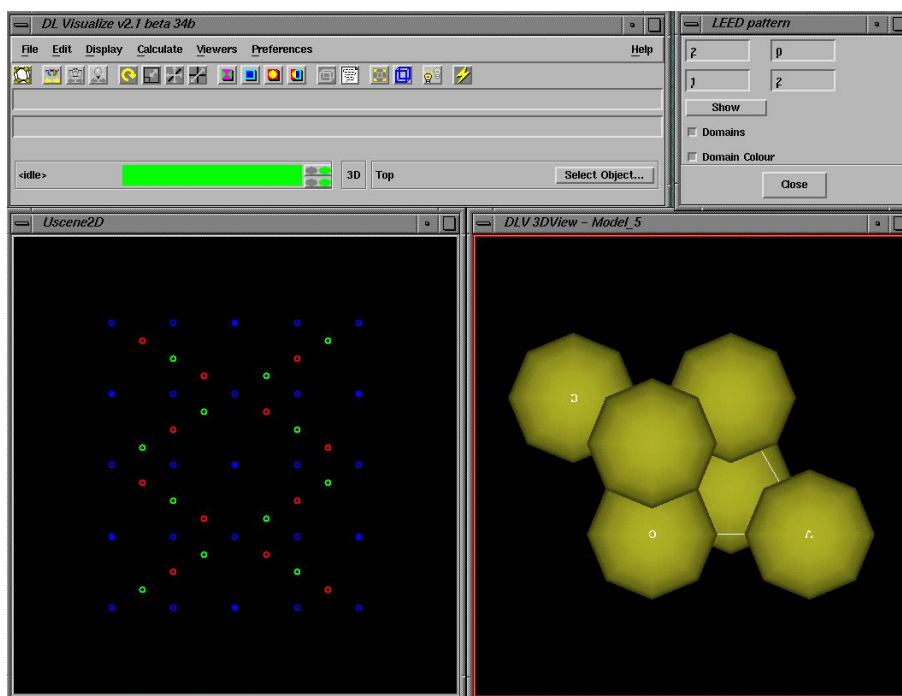


Figure 1: LEED pattern of the $c(2 \times 4)$ Cu(111) Surface demonstrating multiple domains. This pattern is also known as the $(2 \times \sqrt{3})\text{rect}$ reconstruction.

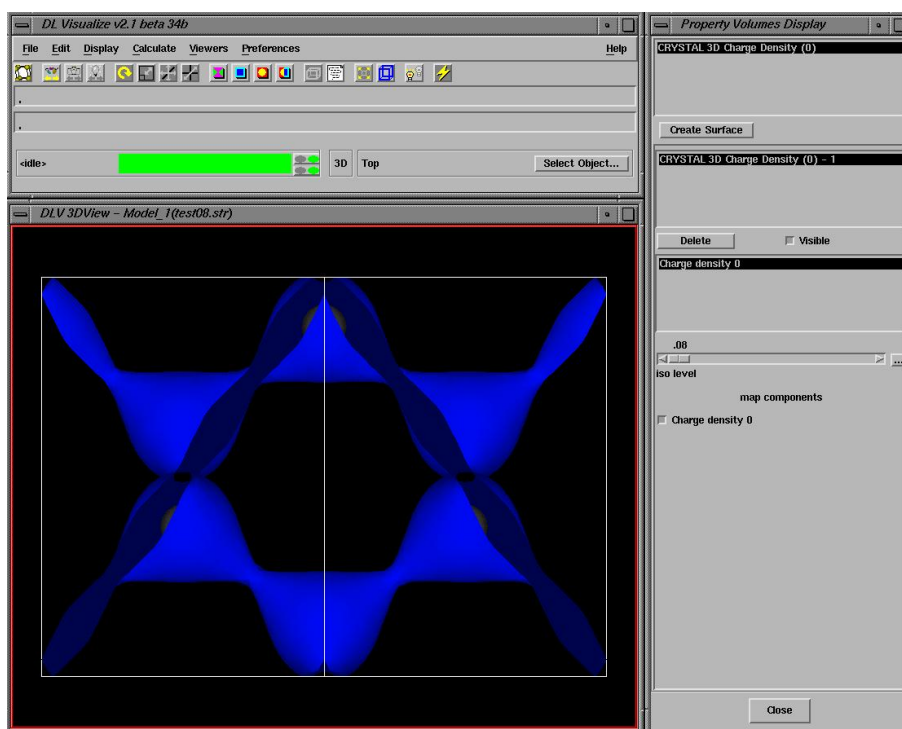


Figure 2: Charge density isosurface plot of bulk silicon.

4 CRYSTAL-2001

CRYSTAL is a flexible package for solving the density functional or Hartree-Fock equations for the ground state wavefunction, energy and properties of periodic systems. The orbitals are expanded in a basis set of atom centred Gaussian functions and thus is capable of very high numerical accuracy for an all-electron (no pseudopotential) description with no shape approximations made to the potential or density.

A new version of CRYSTAL will be released in late 2001 / early 2002. There have been a number of significant developments since the release of CRYSTAL98 in early 1999.

New functionality will include:

- Analytic energy gradients \implies atomic forces.
- Automatic structural optimisation
 - relaxation of internal coordinates and/or unit cell vectors
 - symmetry constrained optimisation
- Support for a wide variety of parallel computers
 - < 64 processors \implies task parallel (using, MPI)
 - > 64 processors \implies data parallel (using MPI and SCALAPack)

In addition the code has been restructured allowing storage for all large data objects to be dynamically allocated. The resultant executable requires about 32 MB of memory for studies of small systems but can also be used in studies of systems with over 1000 atoms.

CRYSTAL is jointly developed by the Theoretical Chemistry Group at the University of Torino and the Computational Materials Science Group at Daresbury Laboratory. Further information is available online at <http://www.ch.unito.it/ifm/teorica/crystal.html>

5 Lab Reports

In a new feature, we present two laboratory reports from members of the working group. We plan to make this an ongoing feature of the newsletter. All members are invited to submit lab reports for inclusion in future issues of the newsletter to ccp3@dl.ac.uk. LaTeX documents are preferred but all major word processing packages can be converted.

5.1 Richard Lambert, Department of Chemistry, University of Cambridge

5.1.1 STUDIES ON TiO₂ AND TiO₂/METAL SYSTEMS.

This area has been attracting interest for some time, from both the surface science and catalysis communities. The gold/TiO₂ system has been the subject of particular attention, thanks largely to the catalytic studies of Haruta et al and the very nice STM data published a while ago by Wayne Goodman and his co-workers. However it has to be said that despite all this effort, very little understanding has emerged in regard to the way in which gold/TiO₂ catalysts actually work, especially in relation to partial oxidation reactions for which the catalyst must be co-fed with an organic reactant, oxygen, AND hydrogen. Why should one have to feed hydrogen to the catalyst in order to get an oxidation reaction to go? There is no consensus about this. All the discussion about quantum size effects and their consequences for the properties of very small gold particles has not generated any insight into how these remarkable gold/titania catalysts actually work.

We are studying the surface chemistry and catalytic behaviour of gold/titania and platinum/titania systems under UHV with respect to the partial oxidation of styrene to the epoxide, as a function of metal particle size. The motivation for this lies in the very striking results produced in Japan, the United States, and by ourselves in regard to the epoxidation of alkenes by practical gold/titania catalysts. This has produced some interesting results, especially in the case of the platinum/titania system where we observe a sudden switch in chemical behaviour from partial oxidation to partial hydrogenation as the platinum metal particle size is changed. In regard to the gold/titania system, we carried out what might be regarded as the ultimate quantum size effect experiment. That is, we left out the gold altogether. What we discovered is something that previously appears to have been overlooked completely. We find that in the complete absence of any kind of metal particle, hydrated titania surfaces exhibit very pronounced catalytic activity towards the partial oxidation of adsorbed alkenes. Isotope tracings studies demonstrate that the oxygen that ends up in the product (in this case acetophenone) originates from the water that was used to create hydroxyl groups on the titania surface; it does not originate from the lattice oxygen of the titania. This striking result may also provide a clue as to why one has to

co-feed oxygen and hydrogen in order to get these metal /titania systems to function as partial oxidation catalysts. One possible role of the hydrogen is that it provides an in situ source of water, in addition to maintaining the surface oxygen vacancy concentration in the titania at a level that enhances the metal/titania interaction.

5.1.2 EPOXIDATION OF STYRENE ON Cu(111) AND (110)

For many years, silver has been regarded as a unique catalyst for the heterogeneous epoxidation of alkenes. However, our fundamental understanding of this system, largely the result of single crystal studies, enables us to deduce what the minimum necessary in sufficient conditions are for a metal surface to act as an effective alkene epoxidation catalyst. These conditions are (i) the presence of oxygen adatoms (as opposed to dioxygen species which have been shown to be catalytically irrelevant) and (ii) the alkene molecule chemisorbed in an appropriate state. In chemical terms this means a π adsorbed alkene as opposed to a σ adsorbed alkene. On this basis, one would predict that oxygenated copper should be an effective epoxidation catalyst, provided that the valence charge state of the oxygen adatoms was appropriate. This in fact proves to be the case. The (111) and (110) faces of copper are extremely efficient in the epoxidation of styrene to styrene epoxide provided that the metal surface is not over-oxidised. NEXAFS experiments were carried out in order to check that there was nothing unusual about the adsorption geometry of the styrene molecule that would cause it to behave in a manner different from other terminal alkenes. We also showed that co-adsorbed Cs is highly effective in increasing reaction selectivity by controlling over-oxidation of the copper surface.

5.1.3 ALKENE EPOXIDATION ON SILVER SURFACES AND THE EFFECTS OF OXY-ANION PROMOTERS

We understand the epoxidation chemistry of silver surfaces rather well. A large amount of work has been carried out on this problem in Cambridge over the last thirty years. Most recently, we have been looking at the way in which the presence of certain oxy-anions on the surface (for example nitrate or sulphate) can enhance reaction selectivity to the point where it is increased from the current state-of-the-art level (around 85%) to nearly 100%. To put this in perspective in technological terms, a sustainable 1% increase in selectivity is worth approximately \$1,000,000 additional profit per year to the operator of a medium-sized ethylene oxide plant. Fast XPS experiments carried out on Ag(100) at Trieste and related work in Cambridge have enabled us to identify and characterise the oxy-anions species that are present under reaction conditions. Currently, we are using isotope tracing methods to determine whether the ultra-selective epoxidation reaction is due to direct oxygen transfer from the oxy-anion to the adsorbed alkene, or whether this process is some how mediated by the metal surface.

5.1.4 AFM STUDIES OF THE GENESIS OF SILVER ON ALPHA ALLUMINA ETHELENE EPOXIDATION CATALYST

Many hundreds of papers have been published describing the properties of vacuum-deposited metal particles on well-defined oxide single crystal surfaces. A great deal of interesting information has been obtained by this approach, and it is commonly stated that one of the principal motivations for carrying out such work is that it sheds light on the properties of heterogeneous catalysts. Of course practical catalysts are not prepared by vacuum evaporating a metal onto an oxide surface. They are prepared on the scale of hundreds of tons at a time by subjecting the oxide to a series of appropriate procedures based on wet chemistry. Therefore it is not obvious that the UHV model systems are necessarily representative of real catalysts in terms of both morphology and stability. Sometime ago Juergen Behm published some very beautiful results for Ag deposition on the (0001) and (11 0) faces of alumina. It was found that the metal particle morphology and stability was essentially the same on both alumina surfaces. Most recently, we investigated the same two systems, but by depositing the silver particles on alumina single crystal surfaces using the same wet chemical route and following exactly the same procedures as are used in the preparation of practical industrial silver-on-alpha-alumina catalysts. We find that the wet chemical route yields completely different systems from those generated by vacuum evaporation under UHV. On the (0001) surface we observe hemispherical Ag particles which are very prone to sintering under oxygen. On the (11 $\bar{2}$ 0) surface we find WIRES which decorate the step edges and extend over many hundreds of nanometres. Furthermore, these Ag wires are much more resistant to sintering under oxygen atmospheres at high temperatures. Clearly, there is a very favourable interaction between Ag and the alumina structure exposed to the step edge. I believe very strongly that this merits investigation by theoretical methods. In principle, we have here the basis for a way forward in rational ab initio design of stable metal-on-oxide catalytic systems. Is there anyone out there who is interested?

Current work on this project involves subjecting these REALISTIC model systems to reaction conditions and observing the changes in morphology and surface composition that occur. We find, for example, that the presence of ppm levels of a chlorine promoter in the gas phase (essential for industrial operation) leads to rapid sintering of the Ag. We speculate that what may be involved here is an Ostwald ripening process in which AgCl acts as the vehicle for inter-particle Ag transport.

5.1.5 ELECTROCHEMICAL PROMOTION OF THIN FILM METAL CATALYSTS

Electrochemical promotion provides an elegant way of modifying the properties of heterogeneous catalyst while they are actually at work. One simply attaches wires to the catalyst film and the electro-active support that is in contact with it. By suitable application of potential differences between the two, promoter species (e.g. alkalis)

maybe pumped to or from the surface of the metal catalyst while simultaneously observing changes in its catalytic behaviour. A particularly attractive feature of these systems is that they are also amenable to post reaction analysis by various electron spectroscopies. For example, in addition to carrying out standard XPS measurements (which are most revealing) we have also carried out photoelectron microscopy measurements at Trieste which have enabled us to determine both the spatial and temporal evolution of the system as the promoter is pumped to and fro. Most recently, we have demonstrated that it is possible to promote Fischer-Tropsch synthesis on ruthenium thin film catalysts contacted with a sodium ion solid electrolyte. Fischer-Tropsch synthesis involves a conversion of CO and hydrogen into long-chain hydrocarbons and oxygenates; it is a process that shows potential for use in the petrochemicals industry because it provides a means of going, for example, from natural gas to fuels or chemical feeds stocks. Thus far, all our work has been carried out at atmospheric pressure. We are now extending these measurements to 30 bar.

5.1.6 OXIDATIVE COUPLING OF METHANE (OCM)

The world is sitting on top of trillions of tonnes of methane. The relatively small amount that is actually used is consumed for one of two purposes; (i) it is burned to provide heating for buildings or (ii) it is burned in power stations to generate electricity. In certain special locations (e.g. Saudi Arabia) it is also burnt to distil seawater to provide all the freshwater required for human activity (not just for drinking but everything else too including flushing the lavatory). OCM provides a potentially very attractive route for the chemical utilisation of methane. The relevant reaction is $\text{CH}_4 + \text{O}_2 \rightarrow \text{C}_2\text{H}_4 + \text{H}_2\text{O}$. In competition with this, and difficult to get around, is the burning of methane to CO_2 and water.

Very recently, we developed a catalytic system that shows considerable promise from the point of view of favourable process economics and hence eventual commercialisation. This makes use of three different metal components supported on α -cristobalite, as opposed to any other form of SiO_2 α -cristobalite is critically important; other forms of SiO_2 lead to extensive burning of the methane. We understand the role of one of the metal components rather well; we partly understand the role of the second metal component; we are working to understand the role of the third metal component. The best formulation we have produced thus far is capable of converting methane to C_2 hydrocarbons with close to 80% selectivity in a single pass. The key point is that 60% of the yield consists of ethylene - which is the desired product. In May 2001, the Saudis announced that for the first time in over thirty years they will allow western oil companies to enter the country in order to carry out exploration recovery and exploitation of hydrocarbon reserves. This does not mean oil (there is no intention to provide access to Saudi oil reserves) but gas, which consists of 95% methane. This is potentially a very interesting development and tips the balance in terms of process economics. We are working to improve our

catalysts yet further and to determine whether they have the degree of robustness required for useful lifetime under the severe conditions that have to be employed ($\sim 1,000$ K).

Richard Lambert, June 2001

5.2 Surface structure and electronic structure: Phil Woodruff, Department of Physics, University of Warwick

This short report is a summary of the main current research activities of Prof. Phil Woodruff at the University of Warwick and at the Fritz Haber Institute in Berlin. The dominant theme of this work is surface structure, mainly associated with atomic and molecular adsorbates on metal surfaces, but with some work on oxides and on silicon, and a growing interest in alloy surfaces and surface alloys the latter being a rather special case of adsorption at metal surfaces. This structural work is pursued mainly with quantitative techniques: scanned energy mode photoelectron diffraction (PhD) based largely on the BESSY facilities in Berlin [1]; normal-incidence X-ray standing wavefield (NIXSW) experiments at the Daresbury SRS and the Grenoble ESRF [2]; medium energy ion scattering (MEIS) using the UK national facility at Daresbury [3]; quantitative LEED at Warwick. In addition, we have a strong interest in the use of STM, especially to try to understand the relationship between adsorbate structures on singular and vicinal surfaces. PhD and NIXSW, in particular, are element-specific structural probes, and one theme we have been trying to exploit more in our recent work is the potential to gain structural information which is also chemical-state specific, by using the chemically-shifted adsorbate core level photoemission signals to monitor the PhD or NIXSW of these specific species. This is an especially powerful capability in cases where coadsorbed species are present on the surface containing the same elements, as in surface chemical reactions. For example, we have used this ability to study the dissociation of methanethiol (CH_3SH) on Cu and Ni surfaces, the reactions (dissociation and disproportionation) of SO_2 on the same surfaces, and photodissociation of PF_3 on Ni(111). A recent short review summarises some of this work [4]. Some recent highlights which give a flavour of this work include:

- PhD studies of CO, NH_3 and NO adsorption on NiO(100) grown epitaxially on Ni(100). There is a dearth of quantitative structural information for adsorbates on oxides, and our results show substantially shorter Ni-N and Ni-C distances than predicted by current ab initio theory, highlighting an important weakness in such theory for this surface.
- Combined PhD and STM studies of the Cu(100) $c(2\times 2)$ -N surfaces; this has long been known to be an unusual system in that one obtains mesoscopically

organised square islands of the ordered phase surrounded by clean surface, but the local structure has been thought to be a simple unreconstructed hollow site. Our results provide clear evidence for an adsorbate-induced symmetry-lowering rumpling of the outermost Cu layer. This rumpling can account for detailed systematics of the inter-island boundaries, and if one assumes it is a result of adsorbate-induced compressive surface stress one may also understand the N-N attraction needed for the island formation.

- A chemical-shift PhD study of N₂ on Ni(100) providing reliable Ni-N and N-N distances through separate PhD data for the two ends of the N₂ molecule, rendered inequivalent by the end-on bonding to the surface.
- Evidence, from MEIS and LEED studies, for a systematic trend for surface alloys to show a smaller surface corrugation than would be expected on the basis of simple effective atomic radii. This is attributed to the same effect of electron depletion at the surface which leads to tensile surface stress at clean metal surfaces [3].

All of these quantitative structural methods, of course, rely on theoretical modelling. In the case of the PhD work, this is based on multiple scattering simulations using a computer code developed for us by Volker Fritzsche which has proved extremely successful. The use of a direct data inversion method (the projection method) also provides some help in indicating the most probably local adsorption sites for many systems. Theoretical modelling for NIXSW is far less computationally demanding; the experimental profiles can be fitted uniquely by a single pair of parameters, the coherent position and the coherent fraction, although further (simple) calculations may be required to interpret these in terms of structural models. The original FORTRAN programs were actually written by me, although we currently perform most of the fitting using IGOR macros written by Rob Jones at the University of Nottingham; these are translations of the FORTRAN codes but benefit from the automated fitting facilities of IGOR-PRO and are thus much more convenient. The main complication in our recent work on NIXSW has arisen because we are increasingly using photoemission monitoring of the photoabsorption (giving access to chemical shifts and light elements) and interpreting these data requires proper account to be taken of non-dipole effects in the photoemission angular dependence; fortunately, we have found a simple way of measuring these non-dipole effects directly [5]. In the case of MEIS, the simulations of the data for different model structures are based on the VEGAS codes originally developed at the AMOLF Institute in Amsterdam, although Paul Quinn, a research student at Warwick, has updated these and implemented them on standard PCs, and introduced a user-friendly front-end for setting up the input files. He has also introduced an automated fitting procedure based on a local gradient method of R-factor optimisation which we have recently tested for Ru(0001)/O chemisorption structures [6].

Our interest in experimental quantitative surface structure determination has recently also led us to start to explore the potential of current DFT codes to model these structures and perhaps gain further insight into their origins. With this in mind I have established a new collaboration with Jim Robinson at Warwick to explore the use of the CASTEP code; we have recently published the results of an investigation of the Cu(111)/Sb and Ag(111)/Sb surface phases with a particular emphasis on the surprising surface stacking fault involved in these phase [7], and are currently completing a study of Cu(111)/CH₃ and Cu(111)/NH₃, all systems we have studied experimentally.

Finally, I should mention a continuing programme of research on surface and thin-film electronic structure in collaboration with Petar Pervan and Milorad Milun at the Institute of Physics in Zagreb. In recent years this has concentrated on angle-resolved photoemission studies on quantum well states in thin films of Ag on V(100). This seems to be a very well-behaved model system which has given us new insight into key aspects of the photoemission process as well as the quantum well states. In particular, we have been studying the influence of the degree of localisation of these states on the photon energy dependence of the photoemission cross-section [8, 9], and most recently on the photoemission peak shapes and the information we can gain concerning electron-phonon coupling at surfaces through such studies [10].

Phil Woodruff, June 2001.

References

- [1] D.P.Woodruff and A.M.Bradshaw *Adsorbate structure determination on surfaces using photoelectron diffraction* Rep.Prog.Phys. 57 (1994) 1029
- [2] D.P.Woodruff *Normal incidence X-ray standing wave determination of adsorbate structures* Prog.Surf.Sci. 57 (1998) 1
- [3] D.P.Woodruff, D.Brown, P.D.Quinn, T.C.Q.Noakes and P.Bailey *Structure determination of surface adsorption and surface alloy phases using medium energy ion scattering* Nucl.Instrum.Methods B in press
- [4] D.P.Woodruff *Chemical-State-Specific Surface Structure Determination* Surf.Sci. 482-485 (2001) 49
- [5] G.J.Jackson, B.C.C.Cowie, D.P.Woodruff, R.G.Jones, M.S.Kariapper, C.J.Fisher, A.S.Y.Chan and M.Butterfield *Atomic quadrupolar photoemission asymmetry parameters from a solid state measurement* Phys.Rev.Lett. 84 (2000) 2346
- [6] P. Quinn, D. Brown, D. P.Woodruff, T.C.Q Noakes, P. Bailey *Structural Analysis of the Ru(0001)(1x1)-O and Ru(0001)(2x1)-O structures by MEIS* Surf. Sci .in press

- [7] D.P.Woodruff and J.Robinson *Sb-induced surface stacking faults at Ag(111) and Cu(111) surfaces: Density-functional theory results* J.Phys.:Condens.Matter 12 (2000) 7699
- [8] P.Pervan, M.Milun and D.P.Woodruff. *Interatomic resonant photoemission from quantum well states in ultra-thin films of Ag on V(100)* Phys.Rev.Lett. 81 (1998) 4995
- [9] M.Milun, P.Pervan, B.Gumhalter and D.P.Woodruff, *Photoemission intensity oscillations from quantum-well states in the Ag/V(100) overlayer system* Phys.Rev.B. 59 (1999) 5170
- [10] T. Valla, M. Kralj, A. Siber, M. Milun, P. Pervan , P.D. Johnson and D P. Woodruff , *Oscillatory Electron-Phonon Coupling in Ultra-Thin Silver Films on V(100)* J.Phys.:Condens.Matter. 12 (2000) L477

6 Programming Tools

CCP3 has recently started to produce a number of introductory guides detailing useful programming tools. These are available online at <http://www.cse.clrc.ac.uk/Activity/ProgrammingTools>.

6.1 Version Management Systems for Code Development: An Introduction to CVS

CVS is a code development tool that, at first site, appears to be a bit of a waste of time. However, it is probably the single most useful tool in software development. Once you start using it you will quickly realise how useful it is, and will wonder how you ever managed without it!

Code availability: <http://www.cyclic.com>

This site contains a number of precompiled versions for a range of operating systems, as well as the source code in case you need to 'do it yourself'.

Version control systems are tools designed to aid program development. They meet an important need in development activities by automated many of the tasks involved. These tasks include maintaining all versions of a program in a recoverable format, merging parallel development tracks into a single version, maintaining version logs detailing changes, and enabling several developers to simultaneous work on different sections of the code.

The principle difference between CVS and RCS is the way in which access to the code by multiple programmers is handled. Within RCS a file being worked on by a programmer is locked preventing other programmers from accessing the same file. Within CVS multiple programmers can have access to the code at the same time!

In both systems, the code is maintained in a single repository. The repository is created (*cvs import*), and the original source code is committed. Subsequently, files are checked out of the repository (*cvs checkout*), modified and checked back in (*cvs commit*). Conflicts created by several programmers editing the same file are flagged at check in time. Each check in creates a new version of the code. (The repository does not store each version. It stores the information needed to generate each version from the original source code - this prevents the repository growing too large). As the code is checked in, the software prompts the users to enter a short description of the changes made to the file, which is stored as a log. Consequently, previous versions of the code are always accessible, and a history detailing the changes in the file is automatically created.

Although CVS is designed to allow multiple users to access the same code I find that the tools available within CVS are more powerful than those within RCS and

hence I use it even for projects on which only I am working.

Typical examples of the problems that can easily be resolved using CVS are:

- A bug has been introduced by a recent edit - what changes were made? This can be checked easily by diff'ing the new version and old version of the code (*cvs diff*).
- I have just accidentally deleted an important file - I can get recover a version from the archive (*cvs update*).
- I am working on a version of the code while someone else is modifying another section of the code to fix a bug. I can update my files easily, and potential conflicts between the two sets of editing will be flagged. If no conflicts are present both versions will be merged automatically (*cvs update*).
- I have worked on a number of files and can't remember which ones. A status command is available letting me know which files have been modified (*cvs status*).
- I modified a file some time ago and can't remember why? A history command is available showing all accesses to the repository together with a log command to examine the comments I made when checking in the file (*cvs log / cvs history*).
- I have released a version of the code. I am now generating new functionality while also supporting the released version. I need to fix bugs in the released version and merge those changes into the current version as well. This is an obvious example of a branch. One branch of the development tree deals with new developments, the other deals with bug fixes. At any point the branches can be merged.
- I have reached a point in the development where I have a reasonably stable version of a code. This can be tagged for ease of later access (*cvs rtag*).

Another useful feature is that code being worked on can be stored on a secure, backed up computer system. Code is then checked out onto local workstations (which are often not backed up!), modified and checked back into the secure central location. CVS can also be used to check out code remotely. We access the CRYSTAL repository from the CRAY-T3E in Manchester during development via a secure shell server (ssh). The developers in Turin also access the code in the same manner.

Hence, the system has tools to aid distributed developers and is also an invaluable aid for the solo code developer. Further introductory material can be found on the cvs website <http://www.cvshome.org/>

Adrian Wander, CLRC Daresbury Laboratory

6.2 Shared Memory Parallelism with OpenMP

OpenMP is a method of parallelizing Fortran and C/C++ codes on shared memory computers. Shared memory computer architectures allow several processors to access memory throughout the system efficiently. This is in contrast to distributed memory systems in which each processor has a localized memory and communication between processors must be imposed explicitly using a language such as MPI.

Useful Addresses:

- <http://www.openmp.org>
- <http://www.mcc.ac.uk/hpc/OpenMP>
- <http://www.mcc.ac.uk/hpc/kilburn/software/OpenMP>

The first site is the home of OpenMP which aims to provide a standardized specification for a set of compiler directives, library routines and environment variables for shared memory parallelism. These have been agreed via collaborative work with interested parties from the hardware and software industries, also from government and academia. OpenMP specification is an informal agreement between vendors and users. The IBM SMP specification, for example, contains customized directives that do not conform to OpenMP in addition to standard directives. These are often less cumbersome than OpenMP directives but are not portable.

The second and third addresses are UK OpenMP sites and include links to training courses in OpenMP directives.

In practice, OMP directives are ‘easy’ to add to a code, and essentially consist of pseudo-comment lines wrapped around local parallelizable sections of code. These directives are ignored by the compiler unless OpenMP is loaded. Shared memory parallelism uses the concept of ‘threads’ and the ‘fork-join’ model. The program begins as a single (master) thread and continues as such until a parallel construct is encountered. The required number of (slave) threads are then created and program statements within the construct are executed in parallel by each thread. At the end of the parallel construct the threads synchronize and only the master thread continues execution. This is in contrast to distributed memory systems in which serial parts of the code are executed independently by each processor.

The main use of OpenMP is to take advantage of the shared memory hardware architecture: implicit data movement, globally addressable ‘cache-coherent’ systems. From a programming point of view, serial codes do not have to be rewritten top-to-bottom to be usable. Compilers may provide some automatic parallelization of straightforwardly written code together with the use of efficiently parallelized library routines: the IBM -qsmp option and esslsmplib subroutine library are examples. Manually, sections of code may be parallelized incrementally with minimal alteration

of structure. As the user becomes more confident in applying OpenMP directives the parallelization may be increased.

The disadvantage of this approach is that efficiency gains are generally lower than can be obtained from a properly written distributed memory code. Most obviously the unaltered serial ‘grand structure’ may not be appropriate for a parallel realization. Each parallel construct requires setting up and shutting down of the parallel environment, plus definitions of which variables remain shared and which variables become temporarily private to each thread. The compiler may not recognise parts of the code as parallelizable. Many ‘clever’ intrinsic functions may not be recognized as parallelizable by the compiler and need to be expanded explicitly into parallel constructs. The piecemeal approach to parallelism may introduce errors and inconsistencies. For example, nested parallelism is allowed in OpenMP with strict rules, however some computers will not support it and revert to serial mode when it is encountered. The localized nature of parallel constructs in sections of code may inadvertently lead to nested parallelism, such as calling a parallelized library routine from within a parallel do-loop, or parallelizing an outer control loop which contains calls to routines which already contain parallel constructs. This may or may not be permissible.

In conclusion, production of a shared memory OpenMP code which is as efficient as a properly written distributed memory code will require at least as much work in rewriting the code as is required for the distributed memory code. However, proper use of parallelizing compiler options and shared memory specific subroutine libraries combined with judicious introduction of parallel constructs will allow the code to take reasonable advantage of the computer architecture for very little effort.

A Fortran Example (this `calc_pi` routine is used in the CSAR/MCC OpenMP training course):

```
program calc_pi
implicit none
integer, parameter :: wp = selected_real_kind (12)
real (wp) :: f, w, sum, pi, a, x
integer :: i, n

f(a) = 4.0_wp / (1.0_wp + a * a)

read (5,*) n
w = 1.0_wp / real(n, wp)
sum = 0.0_wp

!$OMP PARALLEL PRIVATE(x,i), SHARED(w,n) &
!$OMP REDUCTION(+:sum)
```

```

!$OMP DO

do i = 1, n
  x = w * (real(i, wp) - 0.5_wp)
  sum = sum + f(x)
end do
!$OMP END DO
!$OMP END PARALLEL

pi = w * sum
write (6,*) 'pi =', pi

stop
end program calc_pi

```

Using the Manchester CSAR SGI Origin 2000 computer 'fermat,' the MIPSpro 7 compiler command `f90 -mp -O3` and setting `n = 1,000,000,000`, execution time was 53s, 27s, 13s, 7s and 12s (each +/-1s) for 1,2,4,8 and 16 processors respectively. The `-mp` flag allows OpenMP commands to be interpreted. If the OpenMP commands are removed from the program and the flag is replaced by `-ap` (auto-parallelization) the same effect is achieved, however the `-ap` flag only works properly for `-O3`.

Martin Plummer, CLRC Daresbury Laboratory

6.3 Java for Scientific Computing

When examining Java, it is often difficult to see through the hype and buzz-words in order to appreciate what advantages the language would bring to a real application. For scientific programmers this lack of clarity and fears about performance can lead to the language being dismissed as just the latest trend and one that is best avoided.

6.3.1 Getting Started

- Go to <http://java.sun.com> and download the latest version of the Java Development Kit (JDK) for your machine.
- The Java tutorial at <http://java.sun.com/docs/books/tutorial/> provides "trails" for people just starting Java or for those wanting to learn about a particular topic.
- Experiment - Java is a very friendly language and one of the best ways to learn is by attempting to do something and solving problems along the way.

6.3.2 About Java

When it was first released in 1995, Java was described by its creators, Sun Microsystems, as:

A simple, object oriented, distributed, interpreted, robust, secure, architecture neutral, portable, high performance, multi-threaded and dynamic language.

There is clearly a lot more to it than designing irritating applets that clutter up web pages! Many of the features that make Java interesting from the point of view of scientific programming are hidden in this list. Unfortunately these descriptions and explanations involve a bit of Java jargon...

- Object oriented
Java is a fully fledged OO programming language. Whilst it is possible to ignore these features it is much better to fully embrace the OO paradigm. Object orientation is a programming technique very well suited to large applications developed over a long period of time possibly by multiple people. This situation is increasingly common amongst scientific codes.
- Simple
Java is fundamentally a very simple language. The syntax is based on C but people who've had a bad experience with C pointers or string handling shouldn't be put off. If you're moving from a procedure based language such as Fortran then Java is arguably about as simple an introduction to OO (Object Oriented) programming as you can get. Additionally Java comes complete with an enormous set of libraries which allows you to do everything from 3D graphics to network programming to creating easy Graphical User Interfaces with an absolute minimum of effort.
- Interpreted
When you write a piece of code in Fortran, it must be compiled before being run. The same applies to Java but the output of the compiler is not normal machine code but Java byte code. This is in fact a type of machine code, designed to run on a Java Virtual Machine (JVM). The JVM is a small highly optimised utility that reads and executes these simple instructions.
- High Performance
The type of interpreted execution used in Java allows many standard compiler optimisation techniques to be employed in generating the byte code. Additionally JVM technology is improving all the time and "Just-in-time" (JIT) compiler techniques allow for further optimisation and native code generation at run time once all dependencies are satisfied.

Even with all these techniques and constant improvements Java doesn't and won't beat native code for speed of execution. This is a major problem for

many scientific applications but only if you try to do everything in Java. Small critical sections can be left as native code on top of which a graphical user interface or visualisation front-end or whatever can be built using Java.

- **Dynamic**

The interpreted nature of Java allows for a dynamic run-time environment. For example, it is not necessary to think about memory allocation/de-allocation or the size of arrays etc... as this is all handled automatically by the JVM.

- **Architecture neutral and Portable**

A Java application runs on top of a Java Runtime Environment (JRE). A JRE is a combination of a JVM and the standard libraries. Any platform providing a JRE, no matter what the underlying operating system or hardware, is suitable. A Java application is generally shipped in a single JAR file (Java ARchive) thus even eliminating the possibility of filing system incompatibilities.

This feature of Java is one of its main attractions. Existing operating systems providing a JRE include Solaris, HP/UX, Linux, Windows 9x/NT, OS/2, Vx-Works, Inferno, Chorus, AIX, MVS/MP, RiscOS, MacOS, Irix running on architectures such as x86, PPC, ARM, StrongARM, Sparc, MIPS, Alpha. No serious new platform can exist without a JRE. This effectively means that code written in Java is safe from obsolescence.

- **Multi-threaded**

Unlike most languages, Java provides intrinsic support for multiple threads of execution. The implementation depends on the virtual machine and what is provided by the underlying operating system. On a multi-processor system with a JVM that supports native threads, different Java threads will automatically be spread across the different processing elements.

- **Distributed**

An integral part of the the standard java libraries is support for Remote Method Invocation. This is the basis for designing applications that work across completely different machines connected by a network.

- **Robust**

Another consequence of the JVM is the facility to trap errors before they occur at the hardware level. The only way that a Java application can crash in an uncontrolled way is if there is a bug in the JVM. This would be highly unlikely and in general an application level bug will cause a cascade of exceptions to be generated pointing back to the error line in the code. Each exception is an object specific to the nature of the problem. Procedures which can cause the generation of errors e.g. connecting to a remote machine, require that the appropriate types of possible exception be trapped and dealt with in a controlled way.

- **Secure**

The ease by which it is possible to create distributed applications in Java could have led to the proliferation of malicious code. In order to deal with this problem, Java was designed from the outset such that a piece of code, or section thereof, has an associated privilege level. An untrusted piece of code such as an applet downloaded in a web page, for example, is not given access to the local filing system and may only create network connections back to the site from which it was downloaded.

Some of these features may require quite a change in programming style. It should however be obvious that there are clear incentives to make those changes. They should lead to faster application development and more easily maintained code.

6.3.3 Programming tools for Java Developers

- The NetBeans Java development environment is highly recommended. It can be downloaded, free of charge, from <http://www.netbeans.org>.
- Most text editors provide a java mode for syntax highlighting etc...
- For those firmly wedded to emacs there is the Java Development environment for Emacs at <http://www.netbeans.org>.

6.3.4 Useful Java libraries

- [JNL](#) - Java Numerical Library
- Free library from Visual Numerics providing numerical types, linear algebra and statistical functions.
- [Java3D](#) - Java 3D extensions based on underlying native 3D libraries/hardware for excellent performance.
- Many more listed at [JavaNumerics](#).

Daniel Hanlon, CLRC Daresbury Laboratory

6.4 Fortran95 for Fortran77 Programers

Fortran 95 is the current international standard for the Fortran programming language. In itself it is a small revision of the previous Fortran 90 standard, which was a large extension of FORTRAN 77.

On moving from 77 to Fortran 95 the first thing is not to worry! The VAST majority of standard conforming FORTRAN 77 programs are also Fortran 95 programs. One of the prime concerns of the standards committee was to ensure backward compatibility, and as such very little has been removed from the language. What has been removed is generally rarely used and poor practice e.g. The `ASSIGN` statement, real variables for do loops (If you don't know what these are please don't find out, if you do please forget them!). In fact the main cause for incompatibility is if the name of a variable or constant clashes with the name of one the new intrinsic subprograms, and even this, in my experience, is rare.

So why should you wish to move to Fortran 95? Well apart from it being the new standard, and apart from it being a modern, powerful language which allows you to express your programs in a much clearer way, and apart from the language itself providing facilities to aid checking the correctness of your code, some specific examples are:

- Symbols may be up to 32 characters long, allowing such things as variable names to be much clearer (the old cut out the vowels and truncate to six characters is no longer needed). The underscore is also permitted.
- A new, much more flexible source form. You are no longer stuck in the 72 column straitjacket which, when coupled with point one, again improves code clarity
- `Implicit None`. Use it. NOW!
- Parameterized data types and constants. These allow you to portably select the precision for your whole code. For instance in Fortran 77 a Real on many machines occupied 32 bits, while on Crays it was 64 which often caused problems. The use of parameterized data types avoids this entirely.
- An extended range of control constructs. This not only includes such statements as `Do While` and `Select Case`, but also `Cycle` which allows you to skip to the next iteration of a do loop, and `Exit` to leave a loop entirely. Further the `forall` and `where` constructs facilitate parallel programming.
- Array syntax. Array syntax allows operations on a whole array in one statement. For instance if a, b and c are arrays of the same size
 - `a = 0.0` will set the whole of a to zero,

- $a = 2.0 * a$ will double each element of a ,
- $a = b + c$ will set element i of a to $b(i) + c(i)$,
- $a = \text{Sqrt}(b * b + c * c)$ is also permitted.

It is also possible to select subsections of the array, e.g.

$a(3:9) = 2.0 * b(1:7)$ will set $a(3)$ to $2.0 * b(1)$, $a(4)$ to $2.0 * b(2)$ etc.

and even to perform strided operations

$a(1:7:2) = 0.0$ will set elements 1, 3, 5 and 7 of a to zero.

- **Dynamic memory allocation.** Allocatable arrays allow the program to grab the appropriate amount of memory for that array for the current run. This has two advantages
 - No longer do you have to adjust dozens of parameters for a new run of a different size.
 - If a run does not need one of the arrays you need not allocate it, potentially allowing larger sized jobs for a given amount of RAM.
- **Interface blocks** (If you know C these are similar to, but more powerful than, **prototypes**) An interface block tells the calling routine what the correct arguments are for a routine it wants to call. Apart from allowing the compiler to recognize when there is an argument mismatch and so alert the programmer to an error, this is also the basis for some of the more powerful facilities of the language:

Through use of the **Intent facility** it is possible to tell the compiler how the variable will be used in the subprogram allowing extra optimization.

In Fortran 77 it was usually necessary to have to pass not only an array but also its dimensions. Interface blocks make this latter argument unnecessary for it is possible to use some of the new intrinsic functions to find out the size of the array in the called routine.

Interface blocks are how the code implements overloading, and even allows you to create your own operators.

- A number of other features, such as Optional arguments and keyword argument lists are also available.
- **Modules.** There is not enough space here to explain how wonderful modules are! Basically they allow you to encapsulate data and the routines that act upon that data thus helping code organization and clarity. In fact in their simplest form they can even be a glorified **common** block. However they reach their full glory when combined with data hiding using **Private** and **Public**, interface blocks and, if required, derived types (see below). They allow an implementer to provide an interface (e.g. a set of routine calls) for a given

operation to the rest of the program whilst entirely hiding how that operation is carried out. This may not sound very much, but consider:

- You can avoid entirely the possibility of name clashes e.g. between a local variable and a common block
- Say a new and better algorithm for the operation is developed. Modules greatly facilitate the incorporation of this into the code by simply providing a new module with the same interface and NO other changes.

To realize how good modules are you really have to use them!

- Derived data types (**Struct** for C programmers) Derived data types allow you to create your own data types that are more convenient or natural for your code. Further the language has facilities, as mentioned above, to define operations on those types, which when combined with modules allows some extremely elegant code.
- A greatly extended range of intrinsic subprograms. For instance these include portable timers (**System_clock**, **Cpu_time**, **Date_and_Time**), a random number generator, improved character handling facilities, matrix multiplies, dot products, bit handling routines, reduction routines (e.g. **Maxval**) and various inquiry functions to support the new features of the language (e.g. **Allocated** to check in allocatable array is allocated or not)
- A number of other features, e.g. Improved I/O facilities, more edit descriptors, pointers (but they are quite unlike C pointers), recursive subprograms, automatic arrays, array valued functions and zero sized arrays (yes, they do have their uses)

All in all Fortran 95, when compared to Fortran 77, greatly help code clarity, maintainability and portability whilst being almost entirely backward compatible. What are you waiting for?

For more information not a bad place to start is

<http://www.kcl.ac.uk/kis/support/cit//fortran/f90home.html>

which has links detailing not only the language but also what books, on line tutorials, utilities and compilers are available. More specifically for tutorials that offered by the University of Liverpool at

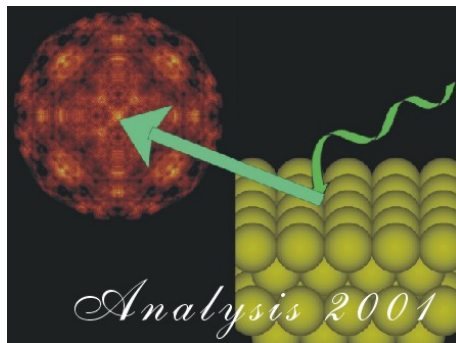
<http://www.liv.ac.uk/HPC/HTMLFrontPageF90.html>

is pretty comprehensive, and as for books I personally like Metcalf and Reid, Fortran 90/95 Explained, Oxford University Press, 2nd edition, 1999, ISBN 0-19-850558-2 though some people consider it best as a reference manual. I have also heard good reports about Kerrigan, Migrating to Fortran 90, O'Reilly and Associates, 2nd ed. Sept.94, ISBN 1-56592-049-X

There is also the news group `comp.lang.fortran` which tends to be a forum with a good signal to noise ratio and the regulars include a number of the standards committee. You might even get a reply from me!

Ian Bush, CLRC Daresbury Laboratory

7 Training Day



Tools for the Analysis and Interpretation of Experimental
Data

A Joint CCP3 and SRRTNet Training Workshop

13th-15th November 2001
CLRC Daresbury Laboratory

Organising Committee

Andrew Fisher (UCL)
Nic Harrison (DL and Imperial College)
John Ingelsfield (Cardiff)
Barry Searle (DL)
Geoff Thornton (Manchester)
Tracy Turner (DL)
Adrian Wander (DL)

International Steering Panel

Massimo Altarelli (Trieste, Italy)
Maurizio Benfatto (Infn, Frascati, Italy)
Paolo Carra (ESRF, Grenoble, France)
Akio Kotani (University of Tokyo, Japan)
Kenji Makoshi (Himenji Institute, Japan)
Rino Natoli (Infn, Frascati, Italy)
John Rehr (University of Washington, USA)
Michel Van Hove (ALS, Berkeley, USA)
Adrian Wander (DL)

This three day workshop is intended for new (and not so new!) experimental and theoretical graduate students working in all areas of synchrotron based research. The workshop will introduce the participants to the modern software tools available for the interpretation and analysis of data and will feature extensive hands-on training in their use. It will provide young research workers with a unique opportunity to learn about the latest programs available to aid their research. The workshop will consist of morning lectures given by international practitioners who will discuss the capabilities and latest developments in the field. The afternoon sessions will feature hands on tutorials in the use of the codes. The outline speaker programme for the workshop is:

- Day 1: Surface Diffraction photoelectron diffraction and surface x-ray diffraction techniques

- Day 2: Photon Interactions with Materials EXAFS, XANES, photoemission and vibrational spectroscopy
- Day 3: Electronic Structure and Processes it ab initio electronic structure calculations as an aid to interpretation

Speakers will include international experts from the USA (ALS, University of Washington, University of Milwaukee) and Europe.

The afternoon sessions will be devoted to demonstrations and tutorials in the use of a wide variety of codes including MSCD (photoelectron diffraction), prAuger (Auger electron diffraction) FEFF and EXCURV (EXAFS/XANES), PHOTON (photoemission), VEGAS (medium energy ion scattering), CRYSTAL and CASTEP (ab initio electronic structure theory). The workshop will make extensive use of the DLVisualise package.

The meeting will be sponsored by CCP3, SRRTNet and the Thin Films and Surfaces Group of the Institute of Physics.

Registration which covers all local costs is 25-00. Places are limited so please register your interest in the meeting as soon as possible.

To register your interest contact CCP3 by e-mail. Alternatively register for the meeting online.

Conference Administrator: Mrs. Shirley Miller, CLRC Daresbury Laboratory, Daresbury, Warrington, Cheshire, WA4 4AD, UK.

Phone: +44 1925 603240 Fax: +44 1925 603634

E-mail: s.miller@dl.ac.uk.

8 News from the Synchrotron Radiation Research Theory Network: SRRTNet

The concept of a global network of theoreticians working on methods for the interpretation and analysis of experimental data collected at synchrotrons was discussed at a meeting in Frascati, Italy in September 1999. Following that meeting, the Synchrotron Radiation Research Theory Network (SRRTNet) was formed (see Synch. Rad. News vol 13 p 17). Membership of the network is open to all interested theoretical and experimental groups. Full details are available on the SRRTNet web pages at <http://www.cse.clrc.ac.uk/Activity/srrtnet>. Funding has been obtained for the European part of the network from the European Union (contract number HPRI-CT-2000- 40014). Similar networks have been established in the USA and Japan, and all of these networks will collaborate to ensure that state of the art software is available to users of synchrotron facilities throughout the world. A number of events of interest to both experimental and theoretical groups are planned for the coming year.

Firstly, the network will hold a conference at the Advanced Light Source in Berkeley, California, USA on the 16th and 17th October. The network conference will be preceded by a meeting on Molecular Environmental Science on the morning of the 16th, and will be followed by a meeting on Excited-State Electronic Structure and Response Functions on the 18th and 19th October - meetings which may also be of interest to network members.

A scientific workshop will be held at Grenoble in early February 2002. The theme of the workshop will be 'Core Level Spectroscopies from Strongly Correlated Electron Systems'. More details of this workshop will be available shortly on the network web pages. This will be the first in an ongoing series of workshops aimed at bringing together leading experimental and theoretical research workers to explore new developments in the field of synchrotron radiation research occurring throughout the world. It is tentatively planned for the 2003 workshop to concentrate on biological aspects of synchrotron radiation, and the 2004 workshop to focus on free electron laser based techniques.

In addition, the network plans to organise a training workshop which is detailed in section 6 of this issue.

Adrian Wander, CLRC Daresbury Laboratory

9 Links

The following web pages may be of interest to readers:

1. CCP3 Related Pages

- CCP3 Home Page <http://www.cse.clrc.ac.uk/Activity/CCP3>
- CCP3 Program Library <http://www.cse.clrc.ac.uk/Activity/CCP3+896>
- CCP3 Jobs Page <http://www.cse.clrc.ac.uk/Activity/CCP3+1075>
- Calendar of Forthcoming Meetings <http://www.cse.clrc.ac.uk/Activity/CCP3+889>
- The DLV Home Page <http://www.cse.clrc.ac.uk/Activity/DLV>
- The CRYSTAL Home Page <http://www.cse.clrc.ac.uk/Activity/CRYSTAL>

2. Other Surface Science Related Groups

- SRRTNet <http://www.cse.clrc.ac.uk/Activity/SRRTNet>
- Thin Films and Surfaces Group of the Institute of Physics <http://www.cse.clrc.ac.uk/Activity/TFSG>
- Solid Surfaces Group of the Royal Society of Chemistry <http://www.rsc.org/lap/rscom/dab/fara016.htm>
- ESCA Users Group <http://www.ukesca.org/home.html>
- UKCP <http://www.cse.clrc.ac.uk/Activity/UKCP>

3. Sources of Useful Software

- The DisCo Home Page <http://www.cse.clrc.ac.uk/Activity/DISCO>
- The NIST Repository <http://http://gams.nist.gov/>
- See also links on the CCP3 pages: <http://www.cse.clrc.ac.uk/Activity/CCP3+1062>

4. Funding Bodies

- The EPSRC <http://www.epsrc.ac.uk>
- The EU Framework 5 Programme <http://www.cordis.lu> <http://www.cordis.lu>

Please e-mail details of useful links to ccp3@dl.ac.uk.

10 Meetings

10.1 Calendar of Meetings and Workshops

These meetings may be of interest for surface scientists. For the latest news, see at the CCP3 webpages <http://www.cse.clrc.ac.uk/Activity/CCP3+889>. To advertise your conference on the web, please send email to ccp3@dl.ac.uk.

- EUROPCAT-V
Fifth European Congress on Catalysis
Ireland, 1st-7th Spetember, 2001
<http://www.ul.ie/cer/EuropaCatV.html>
- ECOSS-20
20th Eurpoean Conference on Surface Science
Krakow, Poland, 4th-7th September 2001
<http://ww.confer.uj.edu.pl/ECOSS20>
- Computer Simulation of Complex Interfaces
Euresco Conference on Electronic Structure of Soilids and Surfaces
Giens, Nr. Toulon, France, 7th-12th September 2001
<http://www.esrf.org/euresco/01/pc01138a.htm>
- Summer School in Molecular Physics and Quantum Chemistry
Jesus College, Oxford, 9th-15th September 2001
<http://physchem.ox.ac.uk/pjg1/summer.html>
- Nato Advanced Studies Institute workshop
Il Ciocco, Italy, 9th-22nd September 2001
<http://cems.alfred.edu/NATO>
- WIRM-2001
International Workshop on Infrared Spectrometry using Synchrotron Radiation and Free Electron Lasers
Porquerolles Island, France, 11th-14th September 2001
<http://www.lure.u-psud.fr/WIRM2001>
- 9th European Conference on Applications of Surface and Interface Analysis
Marseilles, France, 1st-5th October 2001
<http://www.enscp.jussieu.fr/ECASIA/>
- IWSIS-3
3rd International Workshop on Surface and Interface Segregation
Porquerolles Island, France, 7th-12th October 2001
<http://www.crmc2.univ-mrs.fr/confs/iwsis>

- SRRTNet Meeting
Synchrotron Radiation Research Theory Network Conference
ALS, Berkeley, California, 16th-17th October 2001
- Excited-State Electronic Structure and Response Functions
CMSNetwork Meeting
ALS, Berkeley, California, 18th-19th October 2001
www.phys.washington.edu/%7Ejjr/Cmsn/cmsn.html
- IVC-15/ICSS-11 - 15th International Vacuum Congress and 9th International
Conference on Solid Surfaces
San Francisco, California, USA, 26th October-2nd November 2001
- Quantum Simulations of Complex Many-Body Systems: From Theory to Al-
gorithms
Kerkrade, The Netherlands, 25th February-1st March 2002
<http://www.fz-juelich.de/wsqs>
- ICSOS-7
7th International Conference on the Structure of Surfaces
Newcastle, New South Wales, Australia, 22nd-26th July 2002
- ICTF-12
12th International Conference on Thin Films
Bratislava, Slovakia, 1st-6th September 2002
<http://www.savba.sk/sav/fyzi/ictf12>

11 Members of the working group

Chair: Dr. AJ Fisher
Department of Physics and Astronomy
University College London
Gower Street
London
WC1E 6BT
Email: Andrew.Fisher@ucl.ac.uk
<http://www.cmp.ucl.ac.uk/~ajf/>

Prof. D Bird
Department of Physics
University of Bath
Claverton Down
Bath
BA2 7AY
Email: d.bird@bath.ac.uk
[http://www.bath.ac.uk/~pysdb/
home.html](http://www.bath.ac.uk/~pysdb/home.html)

Dr. JA Blackman
Dept. of Physics
University of Reading
Whiteknights
PO Box 217
Reading
RG6 6AH
Email: J.A.Blackman@Reading.ac.uk
[http://www.rdg.ac.uk/Physics/staff/
people/blackman.html](http://www.rdg.ac.uk/Physics/staff/people/blackman.html)

Dr. EA Colbourn
Oxford Materials Ltd
East Grove
Great Busby
Middlesbrough TS9 7AX
E-mail: liz@oxmat.co.uk

Dr. S Crampin
Department of Physics
University of Bath
Bath
BA2 7AY
Email: S.Crampin@bath.ac.uk
<http://www.bath.ac.uk/~pysc/home.html>

Prof. PJ Durham
Daresbury Laboratory
Daresbury
Warrington
WA4 4AD
Email: p.durham@dl.ac.uk
<http://www.cse.clrc.ac.uk/Person/p.j.durham>

Prof. MW Finnis
School of Mathematics and Physics
Queen's University Belfast
Belfast
BT7 1NN
Northern Ireland
Email: m.finnis@qub.ac.uk
<http://titus.phy.qub.ac.uk/group/index.html>

Prof. WR Flavell
Department of Physics
UMIST
PO Box 88
Manchester
M60 1QD
Email: wendy.flavell@umist.ac.uk
[http://chemist.phy.umist.ac.uk/
astaff/wendy.htm](http://chemist.phy.umist.ac.uk/astaff/wendy.htm)

Dr. J Gale
Department of Chemistry
Imperial College of Science, Technology
and Medicine
London
SW7 2AY
Email: j.gale@ic.ac.uk
[http://http://www.ch.ic.ac.uk/
gale/.index.html](http://http://www.ch.ic.ac.uk/gale/.index.html)

Prof. RW Godby
Department of Physics
University of York
York
YO1 5DD
Email: rwg3@york.ac.uk
<http://www-users.york.ac.uk/~rwg3/>

Prof. NM Harrison
Daresbury Laboratory
Daresbury
Warrington
WA4 4AD
Email: n.harrison@dl.ac.uk
[http://www.cse.clrc.ac.uk/Person/
n.m.harrison](http://www.cse.clrc.ac.uk/Person/n.m.harrison)

Prof. S Holloway
Dept IPI Chemistry
University of Liverpool
P O Box 147
Liverpool L69 3BX
Email: stephen@ssci.liv.ac.uk
<http://svr.ssci.liv.ac.uk/~stephen/>

Prof. JE Inglesfield
Department of Physics and Astronomy
University of Wales Cardiff
P.O. Box 913
Cardiff
Wales
CF2 3YB
Email: J.Inglesfield@astro.cf.ac.uk
[http://www.astro.cf.ac.uk/pub/
John.Inglesfield/main.html](http://www.astro.cf.ac.uk/pub/John.Inglesfield/main.html)

Prof. RM Lambert
Department of Chemistry
Cambridge University
Lensfield Road
Cambridge
CB2 1EW
Email: rml1@cam.ac.uk
[http://mria.ch.cam.ac.uk/CUCL/
staff/rml.html](http://mria.ch.cam.ac.uk/CUCL/staff/rml.html)

Dr. WC Mackrodt
Department of Chemistry
University of St Andrews
St Andrews
Fife
KY16 9ST
Email: wcm@st-andrews.ac.uk
<http://ch-www.st-and.ac.uk/staff/wcm/>

Prof. JAD Matthew
University of York
Heslington
York YO1 5DD
Email: jadm1@york.ac.uk
[http://www.york.ac.uk/depts/phys/staff/academic/
matthew/matthew.htm](http://www.york.ac.uk/depts/phys/staff/academic/matthew/matthew.htm)

Prof. D Norman
Daresbury Laboratory
Daresbury
Warrington
WA4 4AD
Email: d.norman@dl.ac.uk
[http://srs.dl.ac.uk/
PEOPLE/D.NORMAN/index.html](http://srs.dl.ac.uk/PEOPLE/D.NORMAN/index.html)

Prof. C Norris
Dept of Physics
University of Leicester
Leicester LE1 7RH
Email: can@le.ac.uk

Prof. RE Palmer
Nanoscale Physics Research Laboratory
School of Physics and Space Research
University of Birmingham
Edgbaston
Birmingham B15 2TT
Email: r.e.palmer@bham.ac.uk
[http://nprl.bham.ac.uk/
About/index.html](http://nprl.bham.ac.uk/About/index.html)

Prof. SC Parker
Department of Chemistry
University of Bath
Claverton Down
Bath
BA2 7AY
Email: S.C.Parker@bath.ac.uk
[http://www.bath.ac.uk/Departments/
Chem/PGProspectus/parker.html](http://www.bath.ac.uk/Departments/Chem/PGProspectus/parker.html)

Prof. JB Pendry
The Blackett Laboratory
Imperial College
Prince Consort Road
London SW7 2BZ
Email: j.pendry@ic.ac.uk

Prof. R Smith
School of Mathematics and Physics
Loughborough University
Loughborough LE11 3TU
Email: R.Smith@lboro.ac.uk
[http://info.lboro.ac.uk/departments/
ma/staff/rogerSmith.html](http://info.lboro.ac.uk/departments/ma/staff/rogerSmith.html)

Dr. GP Srivastava
Dept of Physics
University of Exeter
Stocker Road
Exeter EX4 4QL
Email: gps@excc.exeter.ac.uk
[http://newton.ex.ac.uk/research/
theory/gps/](http://newton.ex.ac.uk/research/theory/gps/)

Dr. S Tear
University of York
Heslington
York YO1 5DD
Email: spt1@york.ac.uk
[http://www.york.ac.uk/depts/phys/staff/academic/
tear/tear.htm](http://www.york.ac.uk/depts/phys/staff/academic/tear/tear.htm)

Prof G Thornton
Surface Science Research Centre and
Chemistry Department
Manchester University
Manchester M13 9PL, UK
email: g.thornton@man.ac.uk
<http://surface.ch.man.ac.uk/pages/surface/home.html>

Dr T Turner
Daresbury Laboratory
Daresbury
Warrington
WA4 4AD
Email: t.turner@dl.ac.uk
<http://srs.dl.ac.uk/sxr/people/tracyturner/index.htm>

Dr. A Wander
Daresbury Laboratory
Daresbury
Warrington
WA4 4AD
Email: a.wander@dl.ac.uk
<http://www.cse.clrc.ac.uk/Person/a.wander>

Prof. P Weightman
Surface Science Research Center
University of Liverpool
Liverpool L69 3BX
Email: peterw@if.ssci.liv.ac.uk
[http://svr.ssci.liv.ac.uk/
people/PWeightman.html](http://svr.ssci.liv.ac.uk/people/PWeightman.html)

Prof. DP Woodruff
Dept of Physics
University of Warwick
Coventry
CV4 7AL
Email: d.p.woodruff@warwick.ac.uk
[http://www.phys.warwick.ac.uk/staff/
dpw/index.html](http://www.phys.warwick.ac.uk/staff/dpw/index.html)