New tools for the analysis of EXAFS: The DL_EXCURV package

Extended X-ray absorption fine structure (EXAFS) is one of the premier tools for the analysis of the local structure of materials. Exciting new experimental developments are underway in the form of micro-focus EXAFS and versatile EXAFS beamlines on the DIAMOND facility. Despite these ground-breaking experimental developments, tools for the analysis of experimental data within the UK have not advanced apace. However, an exciting new collaboration between the EXAFS user group and Collaborative Computational Project 3 is set to change this.

EXAFS, one of the work horse techniques used at synchrotron facilities around the world. It is an important technique on the SRS. It is also seen as a priority for DIAMOND, with three beamlines already planned, including one of the first six to be constructed (Beamline I18 – Micro-focus Spectroscopy). The technique allows local structural and electronic information to be obtained from a diverse range of systems. The user community includes chemists, physicists, biologists, earth scientists and material scientists, with projects ranging from the co-ordination of metals in living tissues to the mechanism of catalysis in the chemical industry.

Within the UK, the principle tool used for the analysis of EXAFS data is the EXCURV program. However, this package has never benefited from direct support by the Daresbury Laboratory and the last official release was EXCURV98 . However, the maintenance and development of a UK package is seen as a priority by the EXAFS user group. Furthermore, previous freely available versions of EXCURV have generally only been accessible via a central server on the Daresbury site, and with the rapid growth in speed and memory of PCs regular users desire a portable version which can be installed in their home university offices.

In 2002 the experimental community approached Collaborative Computational Project 3 to discuss the possibility of establishing direct support for the EXCURV program. These meetings resulted in a new and exciting collaboration that culminated in the development of a grant proposal aimed at modernising, extending and developing the EXCURV package. This proposal was funded by the EPSRC and Stanko Tomic began work as a PDRA on the project in March 2003.

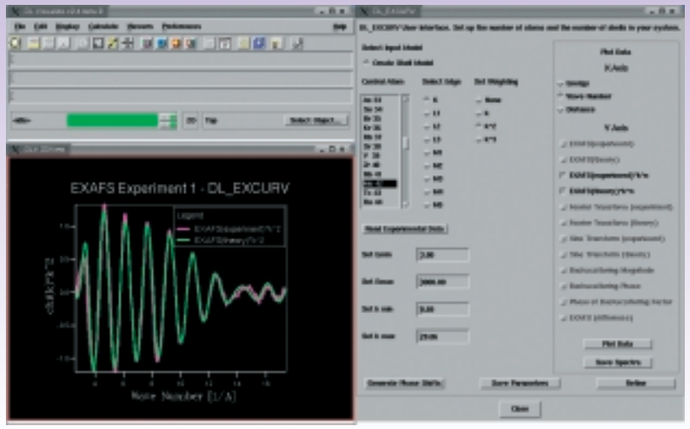

fig 1 *The DLV Interface to DL_EXCURV.*

The old EXCURV package has been re-written in modular Fortran90. System dependencies have been removed and the new code, christened DL_EXCURV,will run on platforms ranging from Windows PC systems through to Unix workstations. In addition, the code has been interfaced to the Daresbury Laboratory Visualize package that provides a powerful environment for the visualisation and manipulation of scientific data. The package also provides a graphical user interface (GUI) to the DL_EXCURV program. DL_EXCURV V1.0 was placed on beta release in late 2003 and test versions, together with the DLV package were installed on end stations at the SRS in early 2004 for user testing and evaluation ***(fig 1)***.

The current version of the GUI allows both single scattering analysis and full multiple scattering analysis of EXAFS data to be performed. Within the single scattering mode the package reports the radius, and occupation, of a series of concentric shells centred around the emitting atom, while in multiple scattering mode a full three dimensional structural determination is performed ***(fig 2)***.

The development of a modular code ensures that future extensions of the code are far easier to achieve. Currently work is in progress to develop improved methods of generating scattering potentials. Traditionally phase shifts have been generated from a superposition of neutral atomic solutions. However, for systems involving substantial charge transfer between the constituent atoms full self-consistent potentials should be utilised. Such potentials will take account of both charge transfer and of the Ewald potential that will be significantly different at the various ionic sites within the crystal. The use of such potentials has already been shown to be of critical importance for the interpretation of low energy electron diffraction (LEED) experimental data for studies of ionic systems where strong charge transfer between the constituent atoms takes place, such as in transition metal oxides .It is highly likely that similar effects will be observed in the analysis of EXAFS data from such systems. It is anticipated that this new feature will be implemented and released in the summer of 2004.

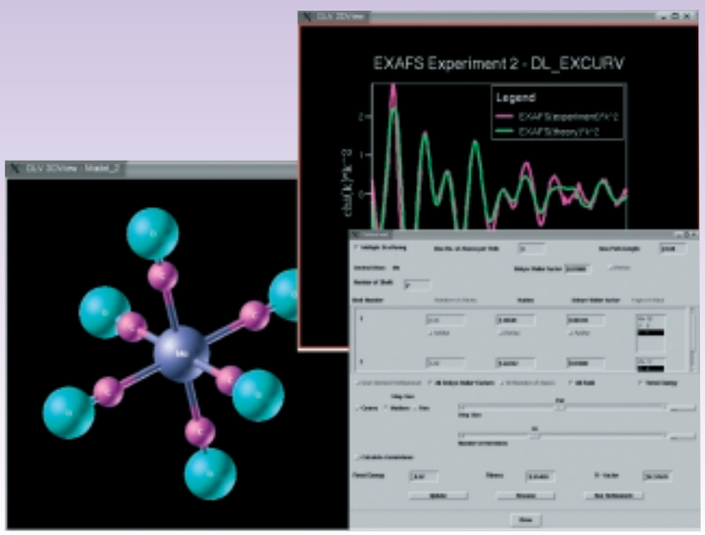

fig 2 *Multiple Scattering Refinement Illustrating the DLV Structural Display.*

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