IRC250610 - Software Developer - Single Crystal Diffraction –

UKRI - Science and Technologies Facilities Council -
Rutherford Appleton Laboratory
Harwell Science Campus
Oxfordshire
UK

Full time, Fixed term 3 Years position

Owned and managed by the Science and Technology Facilities Council (STFC), the ISIS pulsed neutron source at the Rutherford-Appleton Laboratory in Harwell is one of the world-leading facilities that uses neutrons to study materials at the atomic level across a broad range of research areas in chemistry, physics, biology, geology and material sciences, as well as in the engineering and pharmaceutical industries. It supports a national and international community of more than 3000 visiting scientists per year who use the facility for their studies.

The Crystallography Group at ISIS operates nine neutron instruments for diffraction and imaging studies, performing world class powder and single crystal diffraction measurements. Of these instruments, one (SXD) is dedicated to single crystal diffraction, which is recognised as the ‘gold standard’ technique for structural characterisation. The peculiarity of SXD is the ability to work in time-of-flight with polychromatic neutron beams, allowing for the collection of diffraction data over large volumes of reciprocal space at one crystal orientation. However, the treatment of the diffraction data from a pulsed neutron source, and especially the corrections for effects such as extinction and absorption, are more complex than on monochromatic reactor-based instruments. This position will support an ISIS-led project to extend and develop the necessary software for correction and processing of single crystal neutron diffraction data, in order to provide even more accurate and detailed structural information to the SXD user community.

We are looking for a highly motivated and independent scientist to join the Crystallography Group, working with the SXD team to develop the software required to support the scientific programme on the instrument. An ability of working with various programming language (in particular C++ and Python) is essential in order to be able to work with the existing software packages. An understanding of crystallography and diffraction methods is desirable, in order to develop the automation of the data processing flow and the implementation of new routines dealing with complex crystallographic cases (like the treatment of incommensurate structures). An ability to work collaboratively is important, as the successful applicant will be interacting with colleagues at the Diamond Light Source, STFC’s Scientific Computing Department and software teams within ISIS. The appointed candidate will be strongly encouraged to pursue his/her own independent research projects, linked to the scientific programmes within the ISIS Crystallography Group.

List of Duties / Responsibilities.

• Develop, or contribute to the development of, neutron diffraction software for processing of single crystal diffraction data from a pulsed source such as ISIS.
Co-ordinate the development of the analysis software with colleagues in the MANTID software team at ISIS, the Diamond Light Source and within STFC’s Scientific Computing Department.

Provide data analysis support for users of the SXD single crystal diffractometer at ISIS.

Liaise with external networks and facilities (e.g. the European Spallation Source) to ensure the widest use of the software.

Pursue an independent research programme, linked to the activities of the ISIS Crystallography Group.

Present his/her work at national and international conferences and meetings.

**Personal attributes**

**Essential:**
- A PhD, or equivalent degree, in a physical science, engineering or related discipline.
- Solid scientific background in his/her relevant discipline.
- Experience of diffraction methods, using neutrons and/or X-rays.
- Experience of using software for analysis of diffraction data.
- Working knowledge of programming languages (in particular C++ and Python).
- Excellent written and oral English language skills, including good presentation skills.
- Must be capable of working independently and in small teams.
- Potential to develop an independent research programme, linked to the activities of the ISIS Crystallography Group.

**Desirable:**
- Knowledge of single crystal diffraction methods and their data analysis software.
- Experience working with complex data analysis and large data sets.
- Hands-on experience of operating a neutron or synchrotron diffractometer.

For more info please contact:  silvia.capelli@stfc.ac.uk