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| Author: Dr Maximilian Skoda  UKRI, STFC, ISIS, R3 2.03  Chilton, Didcot OX11 0QX  Tel: +44 7500766349  Email: maximilian.skoda@stfc.ac.uk |  |

**ISIS Neutron Reflectivity sample data sets for**

**ExPaNDS Work Package 4 (Data Analysis Services)**

1. **Objective**

To provide a description of the processing used to obtain a ‘fittable’ data set from ‘raw’ data generated by the ISIS reflectometer “INTER”.

1. **Prerequisites**
   1. **Data format**

ISIS ‘raw’ data files (i.e. as saved on disc by the DAE, without any further processing), are provided in Nexus/HDF5 format.

* 1. **Data processing software**

Data processing is performed using the “Mantid” software package.

* 1. **Source type**

The ISIS spallation source is a pulsed neutron source. Data are acquired in time-of-flight (TOF) and are stored as event data sets (sometimes also as histogram data). The INTER reflectometer on Target Station 2 operates at 10 Hz.

* 1. **Instrument set-up**

The INTER reflectometer has a horizontal sample geometry with an incident beam at 2.3° below horizontal. Sample reflection is typically upwards at 2θ angles between 0.5 and 3.0°. There are two sets of horizontal as well as vertical slits used for collimating the beam before the sample and also two vertical and horizontal after the sample. Instrument resolution is dominated by angular divergence defined by the aforementioned slits in the scattering plane. Positional information (which is required for data processing) is stored in the “Mantid” Instrument Definition File (IDF).

* 1. **Information required for data processing**

Instrument specific information, such as distances and detector types, is stored in the “Mantid” IDF. Additional instrument specific information, such as useful wavelength and integration ranges, as well as other default settings, is stored in the “Mantid” Parameters file. Run specific information, such as the scattering angle, run duration, slit settings (gaps) etc is stored in the Nexus file, which can be interrogated by “Mantid”.

1. **Sample data set**
   1. **Sample**

The data presented here were obtained in air as reflectivity from a 3” (75mm) diameter silicon wafer (with native oxide) with a single (unknown) layer on top. The sample forms part of a wider initiative to compare neutron reflectometers world-wide (REF needed).

* 1. **Measurement protocol**

Pre-sample slit settings (vertical gaps) at 0.5° incident angle were 0.412 and 0.267 mm respectively, yielding a resolution of dq/q=0.02 and a footprint of 42 mm.

Four individual “runs” or data sets were obtained by changing incident angle to 0.5, 1.2, 2.3 and 3.0°; Pre-sample slits were scaled linearly with angle in order to keep dq/q and footprint constant. The sample was as aligned in the usual way prior to the measurements. Two “transmission” runs were recorded for data normalisation purposes (see below), using the same vertical gap settings as for the 0.5° sample run (i.e. 0.412 and 0.267 mm). In order to obtain the correct transmission measurement with adequate counting statistics, one of the transmission runs was recorded using horizontal slit gaps as used in the sample run (i.e. 40 and 30 mm respectively for the pre-sample slits) and the other using reduced horizontal gaps of 10 and 7.5 mm respectively, in order to avoid detector saturation. The two transmission runs were the combined as described below.

* 1. **Data processing**

In order to obtain the final “fittable” data set a multi-step normalisation and unit conversion procedure is applied. Details can be found in the “Mantid” documentation (LINK). In short the following steps are necessary:

1. Conversion of TOF data to wavelength and division by monitor integral (4-10 Å default range).
2. Conversion of TOF transmission data to wavelength and division by monitor integral (4-10 Å default range).
3. Combining (stitching) of the two transmission runs using the low wavelength range of the small horizontal slits run and the high wavelength range of the large horizontal slits run. Division of transmission run by its own monitor integral.
4. Division of each of the four angle runs (now in units of wavelength) by the combined transmission run.
5. Conversion of the four angle runs (now normalised for run time and transmission effects) from wavelength to momentum transfer (Q).
6. Combining (stitching) of the four angle runs (now in Q) to form a single dataset with the maximum Q range.
7. Exporting of the “Mantid” workspace (combined run in Q) to ASCII format ready for fitting with a separate software package.
8. **Appendix**
   1. **Relevant meta-information**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Run** | **S1/S2/S3/S4 vertical** | **S1/S2/S3/S4 horizontal** | **Theta /deg** | **Duration**  **/min** |
| INTER00049222 | 0.412/0.267/2.174/2.174 | 40/30/30/40 | 0.5 | 15 |
| INTER00049223 | 0.988/0.638/5.217/5.217 | 40/30/30/40 | 1.2 | 30 |
| INTER00049224 | 1.895/1.224/10.0/10.0 | 40/30/30/40 | 2.3 | 60 |
| INTER00049225 | 2.471/1.593/13.0/13.0 | 40/30/30/40 | 3.0 | 60 |
| INTER00049160 | 0.412/0.267/13/13 | 40/30/30/40 | 0.0 | 30 |
| INTER00049161 | 0.412/0.267/13/13 | 10/7.5/30/40 | 0.0 | 60 |

**Wavelength band used (all runs):** 2.0-15 Å

**Detector type:** 3He tube (0D)

**Resolution:** dq/q = 0.02

* 1. **Mantid reduction short history (complete history as separate file)**

# Child algorithms of ReflectometryISISLoadAndProcess

LoadNexus(Filename='/archive/ndxinter/Instrument/data/cycle\_18\_1/INTER00049222.nxs', OutputWorkspace='TOF\_49222')

ReflectometryReductionOneAuto(InputWorkspace='TOF\_49222', ThetaIn=0.5, WavelengthMin=2, WavelengthMax=14, I0MonitorIndex=2, MonitorBackgroundWavelengthMin=17, MonitorBackgroundWavelengthMax=18, MonitorIntegrationWavelengthMin=4, MonitorIntegrationWavelengthMax=10, FirstTransmissionRun='TRANS\_49161', SecondTransmissionRun='TRANS\_49160', StartOverlap=10, EndOverlap=12, ScaleRHSWorkspace=False, MomentumTransferMin=0.0078343496021074845, MomentumTransferStep=0.014999999999999999, MomentumTransferMax=0.054582042880050204, ScaleFactor=1, OutputWorkspaceBinned='IvsQ\_binned\_49222', OutputWorkspace='IvsQ\_49222', OutputWorkspaceWavelength='\_\_TMP0x8679180', OutputWorkspaceTransmission='TRANS\_LAM\_49161\_49160')

# End of child algorithms of ReflectometryISISLoadAndProcess

# Child algorithms of ReflectometryISISLoadAndProcess

LoadNexus(Filename='/archive/ndxinter/Instrument/data/cycle\_18\_1/INTER00049223.nxs', OutputWorkspace='TOF\_49223')

ReflectometryReductionOneAuto(InputWorkspace='TOF\_49223', ThetaIn=1.2, WavelengthMin=2, WavelengthMax=14, I0MonitorIndex=2, MonitorBackgroundWavelengthMin=17, MonitorBackgroundWavelengthMax=18, MonitorIntegrationWavelengthMin=4, MonitorIntegrationWavelengthMax=10, FirstTransmissionRun='TRANS\_49161', SecondTransmissionRun='TRANS\_49160', StartOverlap=10, EndOverlap=12, ScaleRHSWorkspace=False, MomentumTransferMin=0.018803147212319973, MomentumTransferStep=0.014999999999999999, MomentumTransferMax=0.13100183672511384, ScaleFactor=1, OutputWorkspaceBinned='IvsQ\_binned\_49223', OutputWorkspace='IvsQ\_49223', OutputWorkspaceWavelength='\_\_TMP0x6012a80', OutputWorkspaceTransmission='TRANS\_LAM\_49161\_49160')

# End of child algorithms of ReflectometryISISLoadAndProcess

# Child algorithms of ReflectometryISISLoadAndProcess

LoadNexus(Filename='/archive/ndxinter/Instrument/data/cycle\_18\_1/INTER00049224.nxs', OutputWorkspace='TOF\_49224')

ReflectometryReductionOneAuto(InputWorkspace='TOF\_49224', ThetaIn=2.2999999999999998, WavelengthMin=2, WavelengthMax=14, I0MonitorIndex=2, MonitorBackgroundWavelengthMin=17, MonitorBackgroundWavelengthMax=18, MonitorIntegrationWavelengthMin=4, MonitorIntegrationWavelengthMax=10, FirstTransmissionRun='TRANS\_49161', SecondTransmissionRun='TRANS\_49160', StartOverlap=10, EndOverlap=12, ScaleRHSWorkspace=False, MomentumTransferMin=0.036043783767446338, MomentumTransferStep=0.014999999999999999, MomentumTransferMax=0.25111763593301817, ScaleFactor=1, OutputWorkspaceBinned='IvsQ\_binned\_49224', OutputWorkspace='IvsQ\_49224', OutputWorkspaceWavelength='\_\_TMP0x6012000', OutputWorkspaceTransmission='TRANS\_LAM\_49161\_49160')

# End of child algorithms of ReflectometryISISLoadAndProcess

# Child algorithms of ReflectometryISISLoadAndProcess

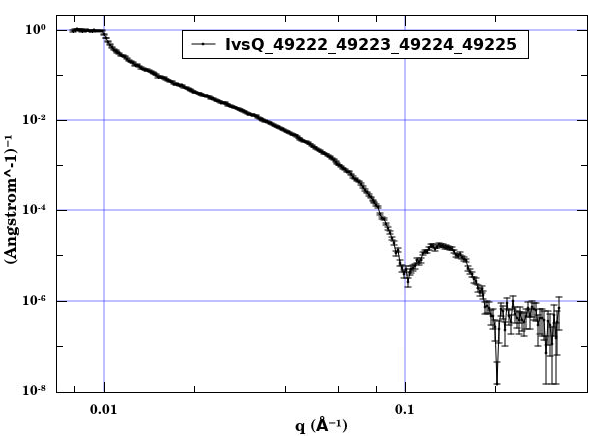
LoadNexus(Filename='/archive/ndxinter/Instrument/data/cycle\_18\_1/INTER00049225.nxs', OutputWorkspace='TOF\_49225')

ReflectometryReductionOneAuto(InputWorkspace='TOF\_49225', ThetaIn=3, WavelengthMin=2, WavelengthMax=14, I0MonitorIndex=2, MonitorBackgroundWavelengthMin=17, MonitorBackgroundWavelengthMax=18, MonitorIntegrationWavelengthMin=4, MonitorIntegrationWavelengthMax=10, FirstTransmissionRun='TRANS\_49161', SecondTransmissionRun='TRANS\_49160', StartOverlap=10, EndOverlap=12, ScaleRHSWorkspace=False, MomentumTransferMin=0.047019235428652495, MomentumTransferStep=0.014999999999999999, MomentumTransferMax=0.32758378866109172, ScaleFactor=1, OutputWorkspaceBinned='IvsQ\_binned\_49225', OutputWorkspace='IvsQ\_49225', OutputWorkspaceWavelength='\_\_TMP0x6c27c00', OutputWorkspaceTransmission='TRANS\_LAM\_49161\_49160')

# End of child algorithms of ReflectometryISISLoadAndProcess

Stitch1DMany(InputWorkspaces='IvsQ\_49222,IvsQ\_49223,IvsQ\_49224,IvsQ\_49225', OutputWorkspace='IvsQ\_49222\_49223\_49224\_49225', Params='-0.015', OutScaleFactors='1.01422,1.06288,1.09925')

* 1. **Final data set**



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