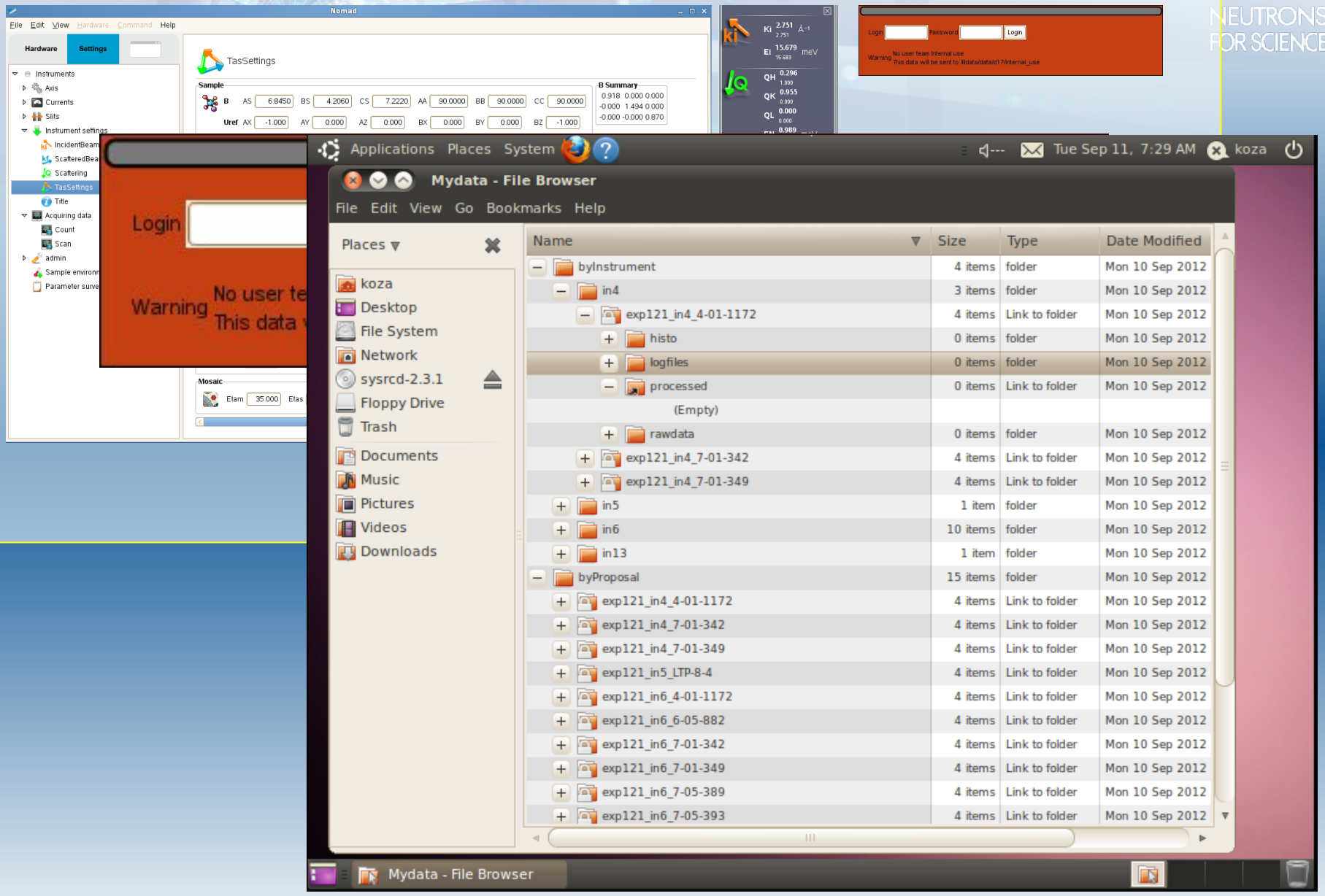
Icat status @ILL

January 2013

Data Policy

- Data Policy implemented since Oct 2012
- Exp. Data Files linked to proposal number
- 1 single account per user
  - Proposal submission system
  - Workstation authentication
  - Data access through NFS(kerberised)/CIFS
  - ICAT authentication

http://www.ill.eu/users/ill-data-policy/


Nomad
File Edit View Hardware Command Help
Hardware
Settings
Instruments
Axis
Currents
Slits
Instrument settings
Scattering
TasSettings
Title
Acquiring data
Count
Scan
admin
TasSettings
Sample
B Summary
Mosaic
Login
Warning
Applications Places System
Tue Sep 11, 7:29 AM
koza
Mydata - File Browser
File Edit View Go Bookmarks Help
Places
koza
Desktop
File System
Network
sysrcd-2.3.1
Floppy Drive
Trash
Documents
Music
Pictures
Videos
Downloads
Name
Size
Type
Date Modified
byInstrument 4 items folder Mon 10 Sep 2012
in4 3 items folder Mon 10 Sep 2012
exp121_in4_4-01-1172 4 items Link to folder Mon 10 Sep 2012
histo 0 items folder Mon 10 Sep 2012
logfiles 0 items folder Mon 10 Sep 2012
processed 0 items Link to folder Mon 10 Sep 2012
(Empty)
rawdata 0 items folder Mon 10 Sep 2012
exp121_in4_7-01-342 4 items Link to folder Mon 10 Sep 2012
exp121_in4_7-01-349 4 items Link to folder Mon 10 Sep 2012
in5 1 item folder Mon 10 Sep 2012
in6 10 items folder Mon 10 Sep 2012
in13 1 item folder Mon 10 Sep 2012
byProposal 15 items folder Mon 10 Sep 2012
exp121_in4_4-01-1172 4 items Link to folder Mon 10 Sep 2012
exp121_in4_7-01-342 4 items Link to folder Mon 10 Sep 2012
exp121_in4_7-01-349 4 items Link to folder Mon 10 Sep 2012
exp121_in5_LTP-8-4 4 items Link to folder Mon 10 Sep 2012
exp121_in6_4-01-1172 4 items Link to folder Mon 10 Sep 2012
exp121_in6_6-05-882 4 items Link to folder Mon 10 Sep 2012
exp121_in6_7-01-342 4 items Link to folder Mon 10 Sep 2012
exp121_in6_7-01-349 4 items Link to folder Mon 10 Sep 2012
exp121_in6_7-05-389 4 items Link to folder Mon 10 Sep 2012
exp121_in6_7-05-393 4 items Link to folder Mon 10 Sep 2012
Mydata - File Browser

Icat is installed!

- Migration from 3.4 to 4.2.2
- LDAP authentication
- TopCat opened: https://icat.ill.eu
- Ingestion Java application rewritten
- Instruments/UserRoles/Proposals ingested
- Dev. of a CLI administration tools (next slide)
- Currently working on the analysis of Nexus files.

ICAT CLI wrapper

- Managing users and groups
- Adding rules, facilities, investigation types, …

```
icat:group:add-rule      Add a rule to a group in ICAT
  Usage: icat:group:add-rule [options]
    Options:
    * -crudFlags
        The CRUD flags. i.e. CREATE, READ, UPDATE OR DELETE
    * -groupName
        The name of the group you want to add the user to
    * -icatPassword
        The ICAT password for the facility admin or data ingestor
    * -icatUsername
        An ICAT facility admin or data ingestor username
    * -what
        What should the rule be applied to?
```

```
hall@hallport:~/workspace/dataimport$ ./run.sh icat:group:add-rule -crudFlags CRU -groupName DataIngestors -icatUsername rootUsername -icatPassword rootPassword -what Investigation
```

```
icat:user:create      Create a user in ICAT
  Usage: icat:user:create [options]
    Options:
    * -icatPassword
         The ICAT password for the facility admin or data ingestor
    * -icatUsername
         An ICAT facility admin or data ingestor username
    * -username
         The username for the user
```

```
hall@hallport:~/workspace/dataimport$ ./run icat:user:create -icatUsername rootUsername -icatPassword rootPassword -username joe
```

```
icat:group:add-user      Add a user to a group in ICAT
  Usage: icat:group:add-user [options]
    Options:
    * -groupName
         The name of the group you want to add the user to
    * -icatPassword
         The ICAT password for the facility admin or data ingestor
    * -icatUsername
         An ICAT facility admin or data ingestor username
    * -username
         The name of the user you want to add to the group
```

```
hall@hallport:~/workspace/dataimport$ ./run.sh icat:group:add-user -icatUsername rootUsername -icatPassword rootPassword -groupName DataIngestors -username icatingestor
```

Citation on ILL raw data

NEUTRONS FOR SCIENCE®
Institut Laue-Langevin

Requested DOI: /10.5291/ILL-DATA.6-05-589

Title: Study of vibrational dynamics in hyperquenched glasses

Authors: C. Angell, H. Schober, T. Scopigno, Y. Yue

Cycle: 20041

Proposal Number: 6-05-589

Numors: 010178 - 010356

Abstract: Using hyperquenching methods on good glassformers it is possible to trap the system in high energy states. The relaxation behavior of the hyperquenched glass is found to be very different from that of the normal glasses. The behavior can not be described at all well by current phenomenological models. The hyperquenched glasses are also very different from the normal glasses in their mechanical properties and in their vibrational properties. The latter are particularly affected in the lowest frequency range. The spectral weight in the hyperquenched glass exceeds drastically that of the normal glass. In this study we will follow the evolution of the low-frequency density-of-states as a function of annealing. We thus obtain information on the vibrational properties of a system confined to a given basin on its energy landscape. Particularly we will be able to determine how the vibrational density-of-states changes with the state of configurational excitation of the liquid.

Dataset(s): ; Author:Yuanzhscho; Numors:010178 - 010356

Sample: Formula: SiO2-CaO with variable relative concentrations
Name: SiO2-CaO with variable relative concentrations

Parameters:

Consistance	N/A	null
Environ Temperature	deg	300 to 600 K
Exp. Energy	Å	4.1 A
Exp. Moment	Å	as given
Exp. Res. Energy	Å	0.2 meV
Exp. Res. Moment	N/A	as given
Size	N/A	7000
Specifications (libelle)	CL	Cryoloop N2
Surface	m^2	3500

Title

Measurement of pressure and temperature dependence of phonon density of states in CaFe2As2

Abstract

The parent compounds MFe2As2 (M=Ba, Ca and Sr) also show pressure-induced superconductivity. In order to understand the role of lattice dynamics in the mechanism of superconductivity it is very important to study the phonon dynamics as a function of pressure and temperature. The pressure induced superconductivity has been found in CaFe2As2 at 3.5 kbar. Phase transition to a collapsed tetragonal phase and superconductivity seem to be related in these compounds. CaFe2As2 is the only compound in the recently discovered FeAs superconductors which shows the transition at a rather low pressure of 3.5 kbar. Our inelastic neutron scattering measurements at ILL indicate that the phonon modes in the Ca compounds show quite different behavior in comparison of Ba and Sr compounds. We expect that low energy phonon modes up to 20 meV would show significant changes in their energy with pressure, which needs to be investigated. The temperature dependence of density of states is required to investigate the changes in density of states across the tetragonal to orthorhombic phase transition as well as to investigate magnetic excitations and for comparison with our measurements on Ca0.6Na0.4Fe2As2.

Download

This data is not currently available to download

Data citation

The recommended format for citing this dataset in a research publication is in the following format: **[author]**, **[date]**, **[title]**, **[publisher]**, **[doi]**

Instrument

IN6 IN4

Data has been collected on the IN6 instrument

Metadata

DOI
doi:10.5291/ILL-DATA.7-02-110

Authors
BRUECKEL Thomas, CHAPLOT Samrath, MITTAL Ranjan, NAVEEN KUMAR Chogondahalli M, ROLS Stephane, SCHOBER Helmut, SU Yixi, TEGEL Marcus

Publisher
Institut Laue-Langevin

Publication year
2011

Cycle(s)
20084
20091

Proposal number
7-02-110

Date of experiment
17-03-2009

Experiment parameters

Environment temperature
At 300 K IN6

Experiment energy
upto 50 meV

Experiment res energy
60 micro eV

Sample parameters

Formula
CaFe2As2

Consistence
polycristalline

Mass
15000

Size
3000

Surface
400

Space
I4/mmm

Unit cell A
3.887

Unit cell B
3.887

Unit cell C
11.758

Alpha
90

Beta
90

Gamma
90

Container
Pressure cell and cylinder

Next goals/Backlogs

- PANData software integration
- Data Mining coupling
- Umbrella authentication

Issues & Questions

- An investigation cannot be related to many instruments
- Many proposals and one dataset
- Internal ID of the proposal system – link?
- Synonym table – inside ICAT or external?
  - User looking for CU vs Copper
  - Different abbreviations for temperature