inserexs user guide

Last update: 12/12/2022

1. Program description:

inserexs has been written in Python 3.9 language and has been tested on Windows 10 and Ubuntu 20.040 LTS. It has also been adapted for Mac users. *inserexs* consists of three different modules and a graphic interface.

- main.py: backbone, direct exchange with interface.
- intensity module.py: module for the calculation of the reflection intensities.
- sensitivity module.py: module for the calculation of the reflection sensitivities.

2. General set-up:

For the correct running of the *inserexs* code, the following Python packages (not included in the standard version of Python 3.9) should be installed. The versions used in the conception and trial of the code are indicated.

- numpy – 1.21.5
- matplotlib – 3.5.1
- PyQt5 – 5.14.4
- promptlib – 3.0.20
- threading – 4.1.0
- scipy – 1.10.11
- pandas – 1.4.2
- sympy – 1.10.11

The three .py modules that compose the code, as well as the interface and the icon image, should be present in the same directory. Furthermore, two additional directories should be present:

a. A "FDMNES" folder, from where the fdmnes code will be launched. The "fdmnes_win64.exe" file should be present in this folder for Windows systems, and the "fdmnes_linux64" file for Linux. The fdmnes software should be downloaded from its original source: Download - The FDMNES project FDMNES download: package with executables, manual and input file examplesThe FDMNES project (cnrs.fr) and then moved to this folder. Another option would be to explicitly indicate the location in the code itself.

UPDATE: for linux users, an error can occur if FDMNES does not have the proper permissions. If an error arises, please check that FDMNES can be run normally.

b. A "Sasaki anomalous" folder, which contains the data from the International Tables of Crystallography that are needed for the calculation of the atomic scattering factors.

Some folders will be automatically created inside the "FDMNES" folder for the communication of the *inserexs* program and fdmnes. This folder will also contain the "FileResults" folder which stores all the output files for the simulation as well as the final "Sensitivity vs. Intensity" plot image.

3. Running instructions

i. Once the main.py module is executed, the interface windows should pop up.

ii. From there, the user must press the "Load .cif file" button. A pop-up window will then appear, letting the user choose the .cif file which contains all the crystal information. The requirements that the .cif file must respect are indicated in part…

- If the user wants to change any crystallographic data, they can do it from the interface. After any modification the "Update" button should be pressed.

iii. A maximum value for the h, k and l Miller parameters of the generated reflections should be introduced. The default value (2) is useful for quick simulations but might be too small for real uses.

- If the user wants to consider the forbidden reflections (some of them active in REXS), they can check the "Include forbidden reflections" checkbox.

iv. After pressing the "Fetch active reflections" button, the reflections are generated.

v. From the "Atomic information" table, the parameters of interest (atomic positions or occupation) should be chosen. If the chosen parameter does not respect the crystal symmetry (e.g. refinement of a fixed special position) fdmnes will laterly raise an error.

vi. The different conditions for the FDMNES simulations should be filled in: the energy start, the energy step and the energy stop around the edge. The edge for simulation should be chosen in the "Atom" table. The default parameters are suitable for quick simulations but longer ranges are more convenient for most simulations.

- The user has the possibility to make all the chosen parameters vary simultaneously (coupling) or independently (not coupling) by checking the "Couple refinement parameters" checkbox.

vii. The "Launch simulation" button will run the FDMNES program.

viii. Once the simulation process finishes, the "Sensitivity vs. Intensity" button makes a plot of the calculations and outputs a .png file in the "FileResults" folder.

4. Data input

As previously mentioned, the data input takes place in the form of a .cif file. *inserexs* has been tested in a wide range of .cif file of different materials, space groups, document styles and sources. A showcase .cif file could be the following (in red, the mandatory parts for the crystal information detection):

#--

#$Date: 2017-10-06 19:24:22 +0300 (Fri, 06 Oct 2017) $

#$Revision: 201816 $

#$URL: file:///home/coder/svn-repositories/cod/cif/9/01/46/9014668.cif $

#--

This file is available in the Crystallography Open Database (COD),

http://www.crystallography.net/. The original data for this entry

were provided the American Mineralogist Crystal Structure Database,

http://rruff.geo.arizona.edu/AMS/amcsd.php

The file may be used within the scientific community so long as

proper attribution is given to the journal article from which the

data were obtained.

#

loop_

_publ_author_name

'Xiao, C. J.'

'Jin, C. Q.'

'Wang, X. H.'

_publ_section_title

;

Crystal structure of dense nanocrystalline BaTiO3 ceramics

Note: phase T (tetragonal)

;

_journal_name_full 'Materials Chemistry and Physics'

_journal_page_first 209

_journal_page_last 212

_journal_paper_doi 10.1016/j.matchemphys.2008.01.020

_journal_volume 111

_journal_year 2008

_chemical_compound_source Synthetic

_chemical_formula_sum 'Ba O3 Ti'

_space_group_IT_number 99

_symmetry_space_group_name_Hall 'P 4 -2'

_symmetry_space_group_name_H-M 'P 4 m m'

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 90

_cell_length_a 3.9988

_cell_length_b 3.9988

_cell_length_c 4.0222

_cell_volume 64.317

_database_code_amcsd 0018579

_exptl_crystal_density_diffrn 6.021

_cod_original_formula_sum 'Ba Ti O3'

_cod_database_code 9014668

_amcsd_formula_title BaTiO3

loop_

_space_group_symop_operation_xyz

x,y,z

-y,-x,z

-y,x,z

x,-y,z

-x,-y,z

y,x,z

y,-x,z

-x,y,z

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

Ba 0.00000 0.00000 0.00000 0.19600

Ti 0.50000 0.50000 0.50210 0.01800

O1 0.50000 0.50000 -0.01530 0.01700

O2 0.50000 0.00000 0.51300 0.01100

```
loop_
_cod_related_entry_id
_cod_related_entry_database
_cod_related_entry_code
1 AMCSD 0018579
#--------------------------------------------------------------------------
```

For the space group, both the group's number or the name are accepted. The former is recommended in most cases to avoid any style difference. If a setting is needed, it should be indicated after a semi-colon (e.g. 227**:2**)

5. Additional information

A more detailed description of the code and some general examples will be shown in a yet-to-come publication. This user guide will be expanded with visual examples when this publication is accepted.