# Benchmarking the neutron inelastic scattering model in NCrystal

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# Introduction to NCrystal

NCrystal is a fusion between harmonic, quasi-harmonic scattering cross section models and highly optimised Monte Carlo sampling methods. It supports three and only three types of user operations for single- and poly-crystals,

1. defining a crystalline material and its orientation.
2. calculating the total scattering cross section for a given incident energy and momentum direction.
3. sampling the scattered neutron energy and momentum direction.

NCrystal is designed to be,

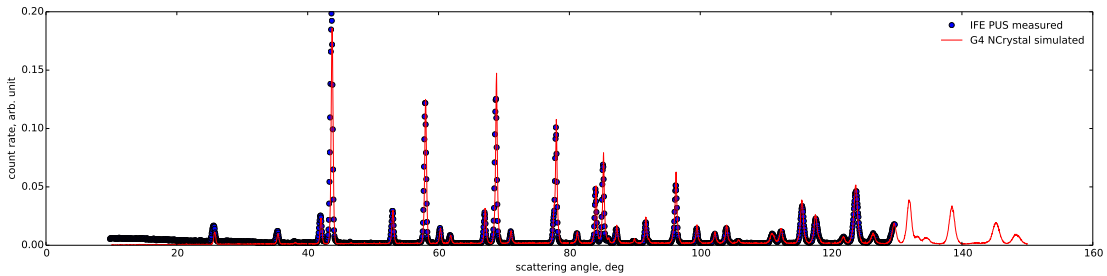
1. clean and portable. No external dependence.
2. minimalist. Less than 10 lines (3 lines in the case of powder) of user code to reveal its full power.
3. ab initio. No tunable parameter.
4. multilingual. C and python bindings.

It is primarily developed by X.X. Cai and T. Kittelmann. Significant contributions have been received from E. Klinkby in the process of theory development. It will be heavily used by members of the ESS detector group to gather early user feedback.

It is currently available to users of the ESS detector group coding framework. It will be made available in the official releases of Geant4 and McStas. The open-source stand-alone distribution will also be made available.

# Progress of our validation work

The coherent elastic model has been bencharmed against data from the PUS powder diffractometer at IFE Norway. We simulated the full-scale instrument from the reactor moderator boundary to the instrument detectors in Geant4, including a Ge-511 monochromator and an alpha-$Al_2O_3$ powder sample [1].




This talk is confined to the benchmark of the NCrystal inelastic model, which can sample over 1.3 million/s/CPU scatterings [2] directly from an $S(Q, \omega)$ table based on a rejection method. It can be initialized by

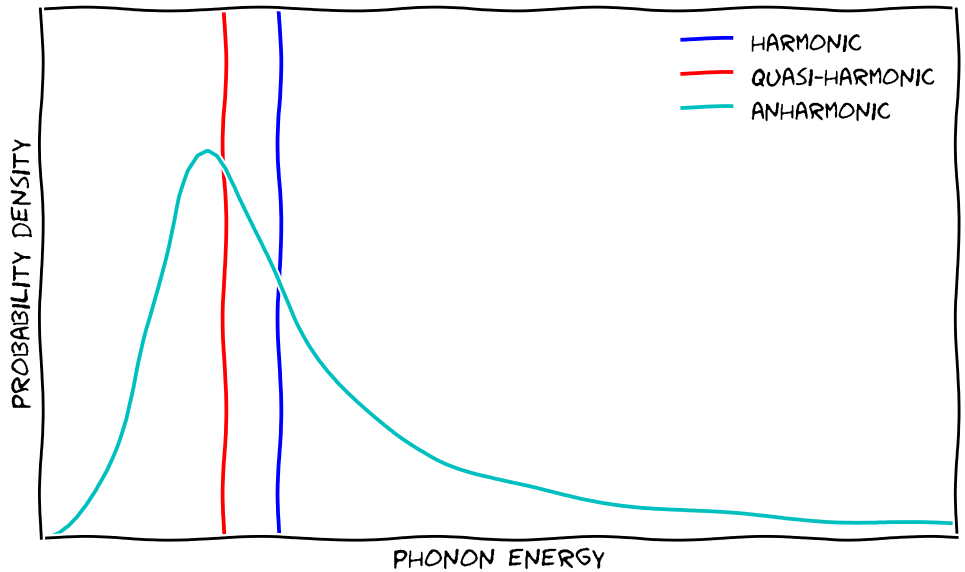
1. an $S(Q, \omega)$ table from a measurement of any material
2. an $S(\alpha, \beta)$ table from ENDF ( typically in $\sim$150ms)
3. vibrational density of state using the NCrystal static model (typically in $\sim$1.5s)
4. model Grüneisen parameters and thermal expansion data using the NCrystal QHA model (typically in $\sim$1.8s)

[1] experimental data are kindly provided by Dr. Magnus H. Sørby

[2] speed estimated in a late 2014 main-stream laptop

# Method

The energy of a phonon in the views of three different theories.

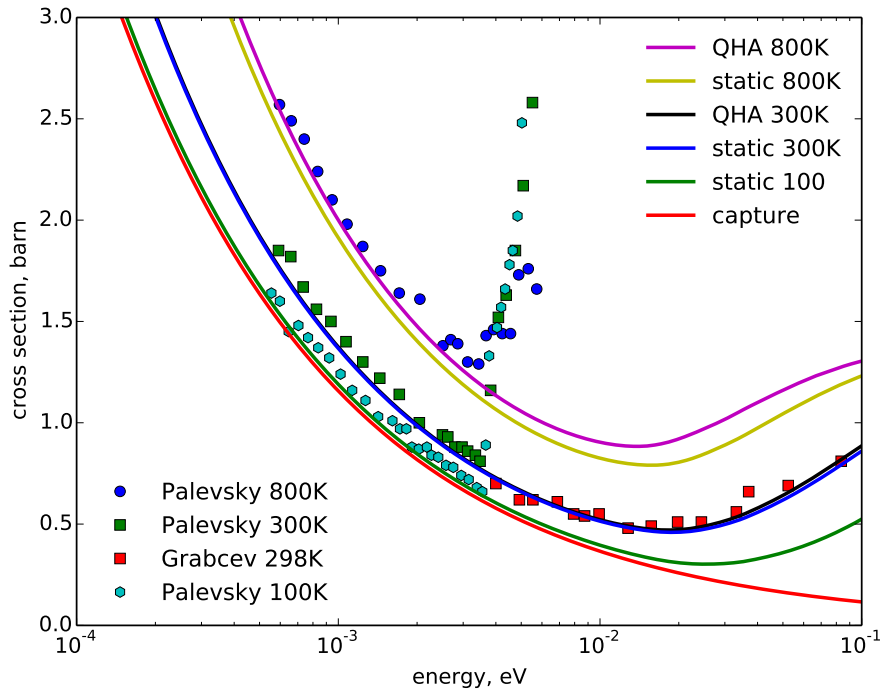



- Modern ab initio methods provide a powerful mean to compute phonon characteristics and mode grüneisen parameters from first principles.
- NCrystal supports the harmonic and quasi-harmonic theories.

# The static and QHA models in NCrystal

- We call the model that is based on the harmonic theory [3] the static model, the equivalence of which can also be found in NJOY.
- We call the model that is based on the quasi-harmonic theory the QHA model. The input of the model are the mode Grüneisen parameters and thermal expansion data.

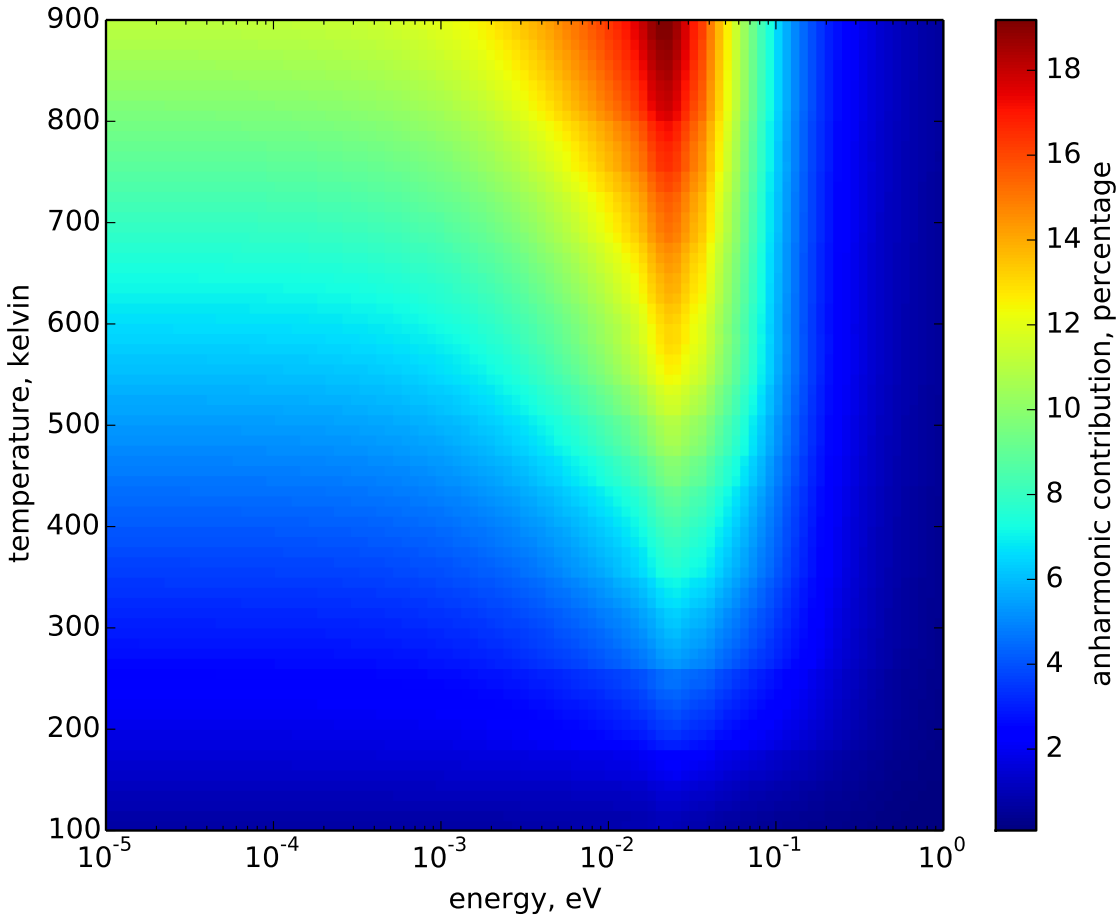
Calculated **total** cross section of single crystal Al at 100K, 300K and 800K are compared with data compiled in EXFOR.




[3] Alf Sjölander, Ark. Fys., 1958, 14, 315-371

# The static model underestimates cross section at high temperature

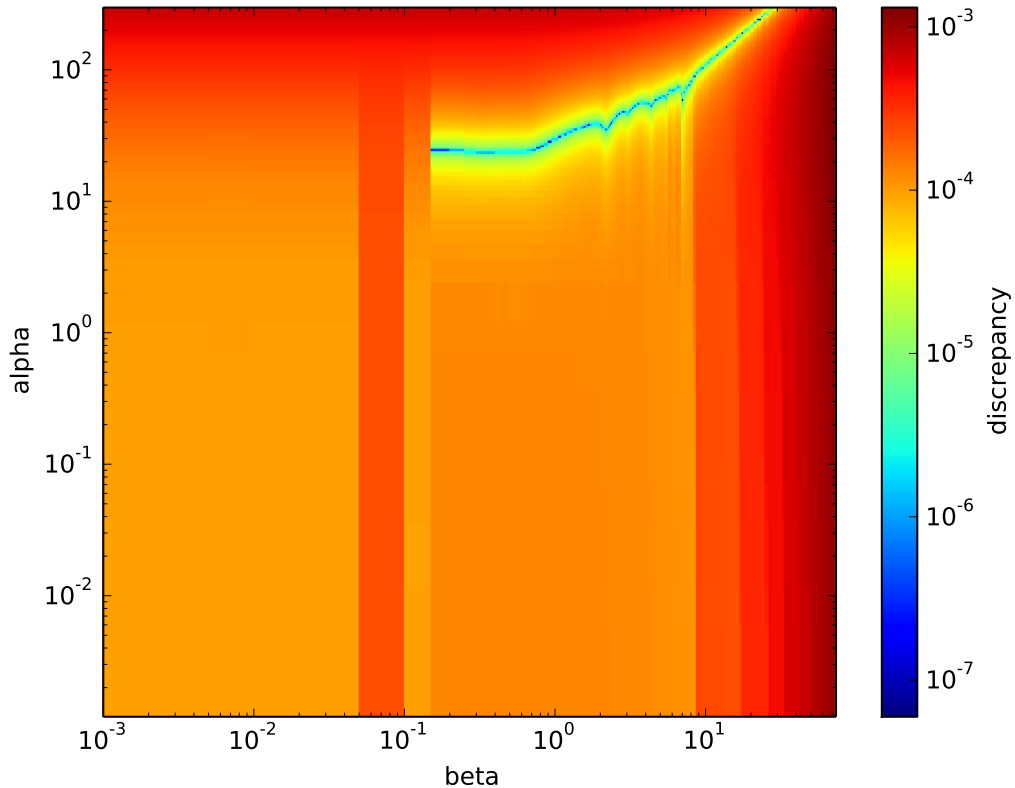
The underestimation of the **inelastic** scattering scattering cross section in Al by the static model.



# Benchmarking the phonon expansion calculation

## against NJOY

We run NCrystal and NJOY using the same density of state in graphite at room temperature, the discrepancies between the calculated $S(\alpha, \beta)$ are typically less than 0.1%.

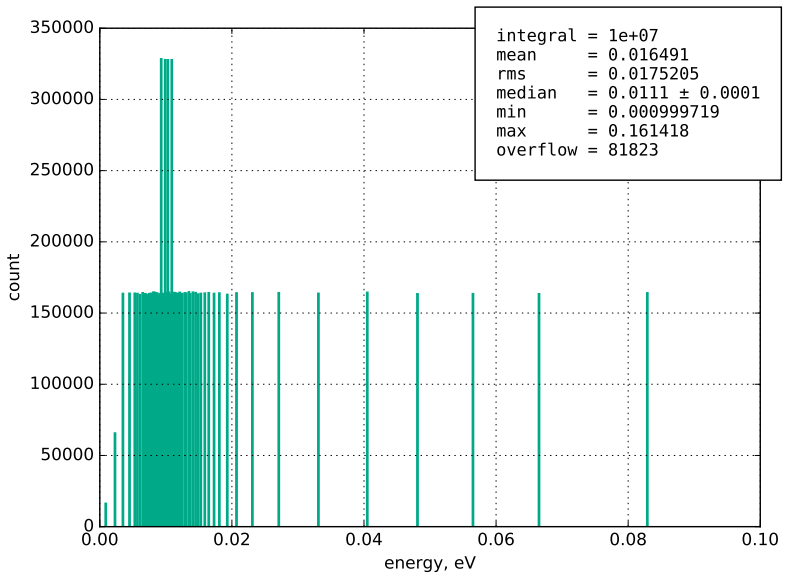



We noticed about 1.5% discrepancies in the integral cross sections in the 1/v energy region. As the method NJOY used to check the convergence of the integral is unknown to us, it is difficult for us to trace down the sources. But such discrepancies are comparable with, if not much smaller than, the measurement uncertainties in EXFOR.

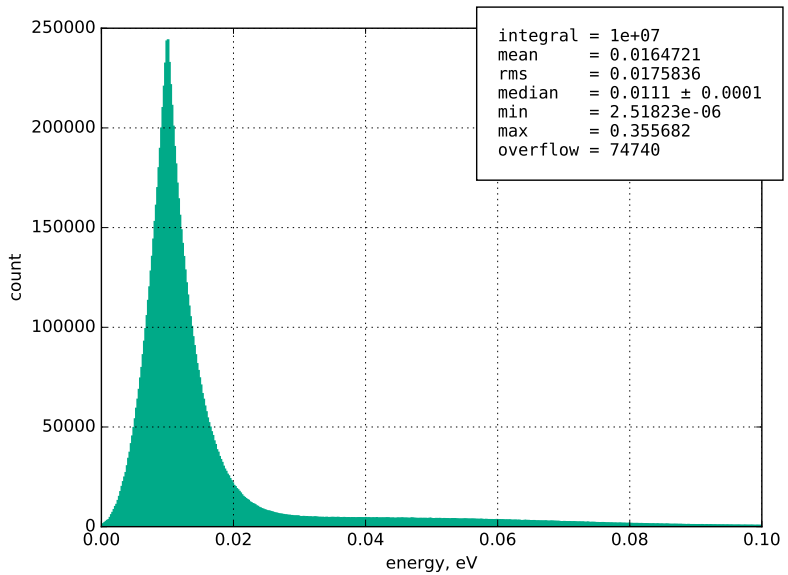
# Benchmarking the scattering kernel sampler

## against the ace model, ENDF/B-VII water kernel, scattered energy distribution

We denote the sampling from a discrete ACE formated file as the ACE model, and the sampling from an $S(Q, \omega)$ table as the COTS model. Example of sampled energy distributions of 10 million incident 0.1 $\mathrm{eV}$ neutrons are shown below.




(a) ACE, mean energy 16.491 $\mathrm{meV}$

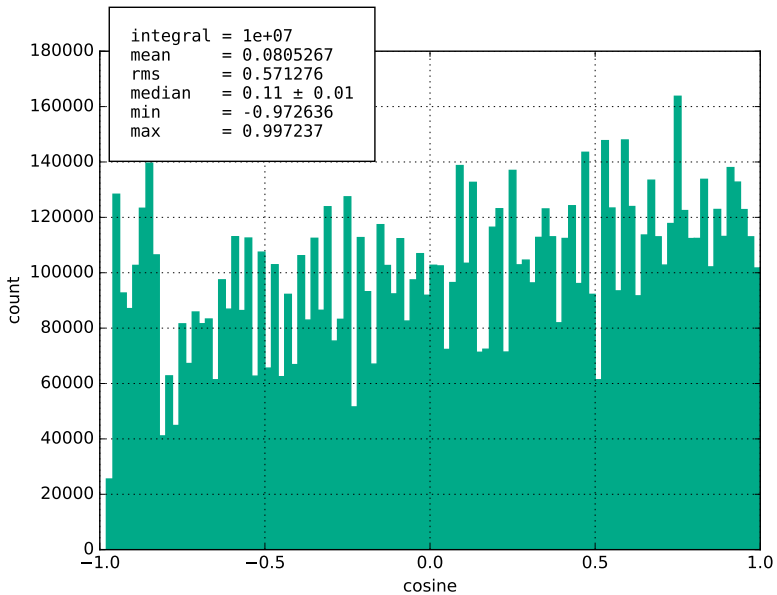



(b) COTS, mean energy 16.472 $\mathrm{meV}$

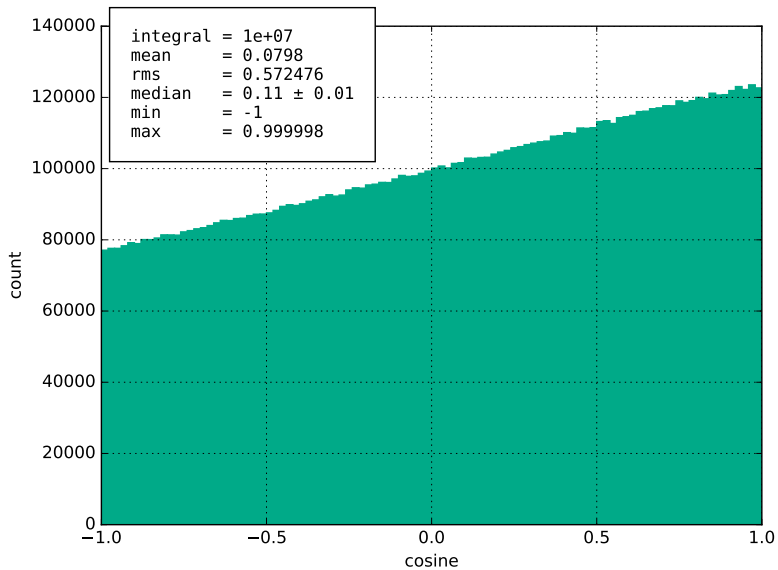
# Benchmarking the scattering kernel sampler

## against the ace model, ENDF/B-VII water kernel, scattered angular distribution

Example of sampled cosine angle distributions of 10 million incident 0.1 $\mathrm{eV}$ neutrons are shown below.




(c) ACE, mean consine angle 0.0805

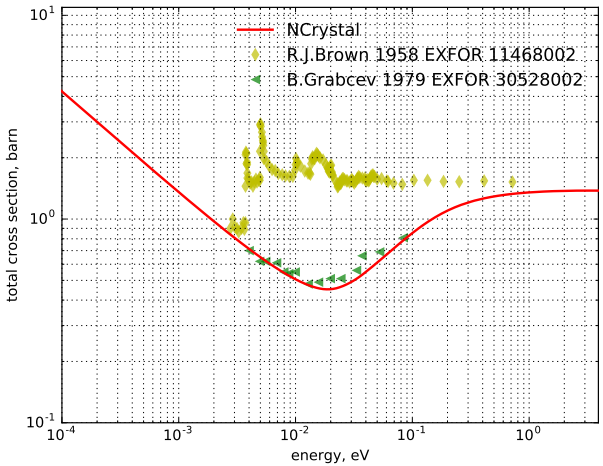



(d) COTS, mean consine angle 0.0798

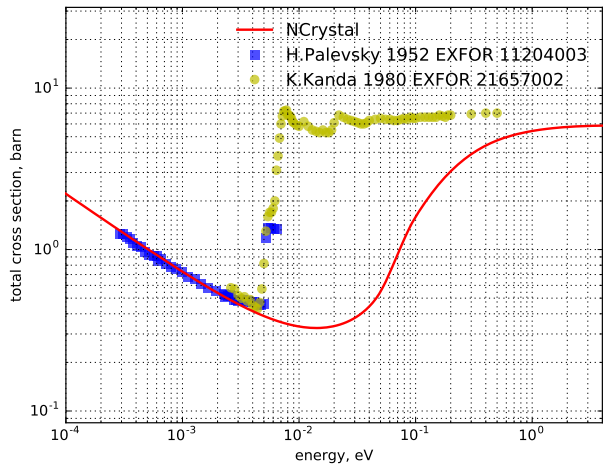
# Benchmarking the static model [4]

## elemental crystals, against data

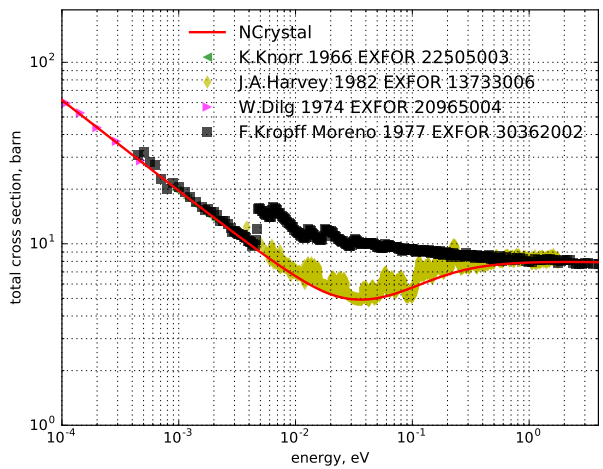
Comparisons with data compiled in EXFOR at room temperature, which is far below the melting point of the materials.

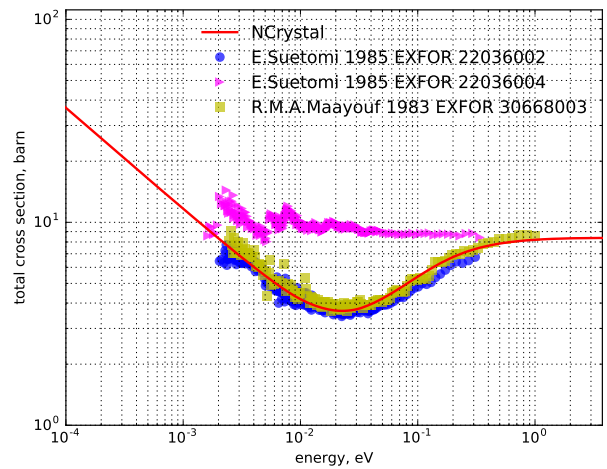



(a) Al




(b) Be

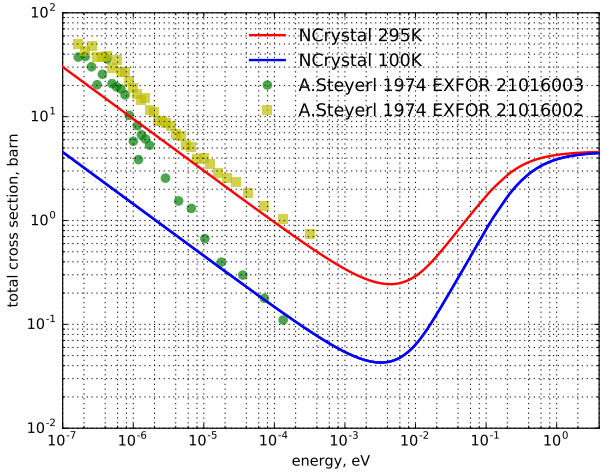


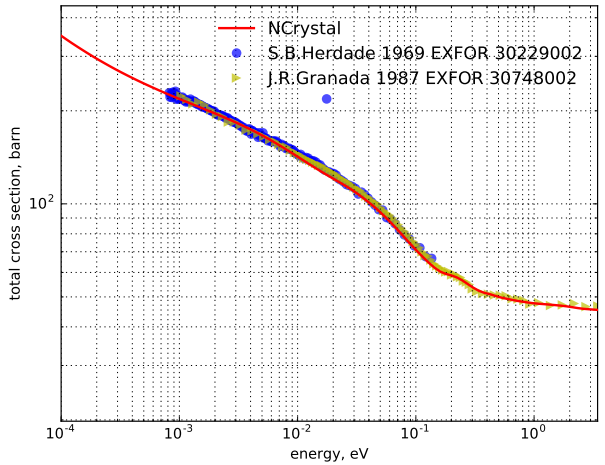
# Benchmarking the static model

## general crystals, against data

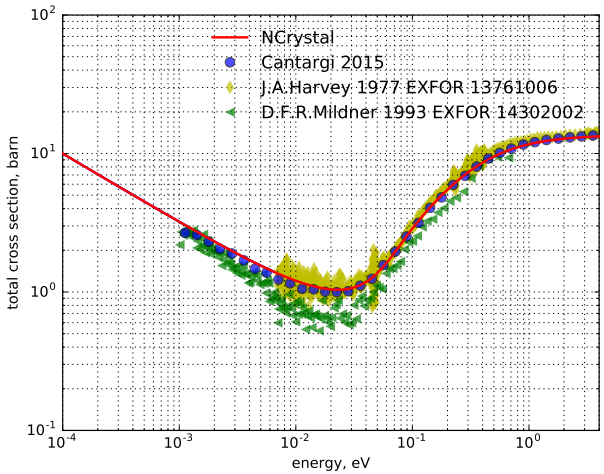
The important van der Waals forces in graphite and polyethylene can be treated satisfactorily. Corundum and MgF2 are promising neutron filters.



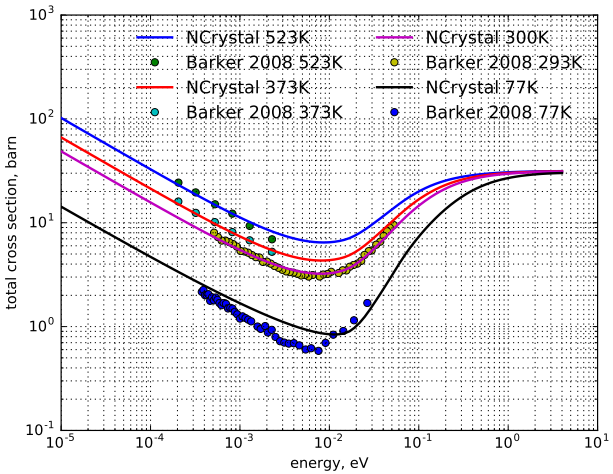

(e) graphite




(f) polyethylene




(g) alpha-Al2O3 (corundum)

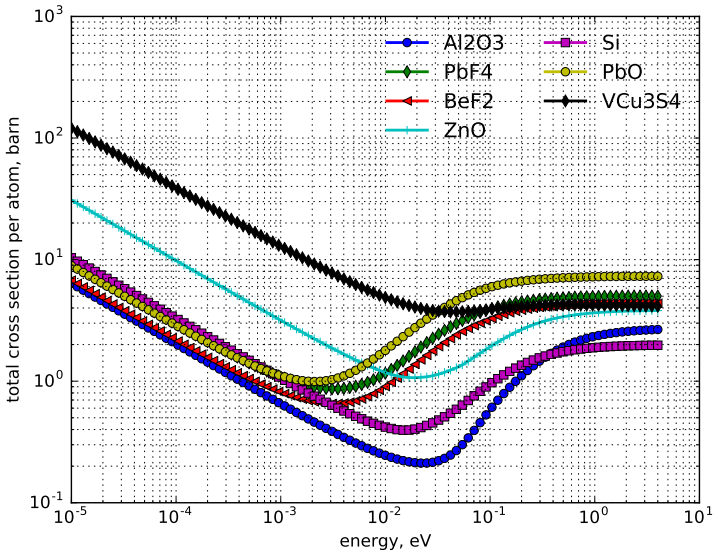


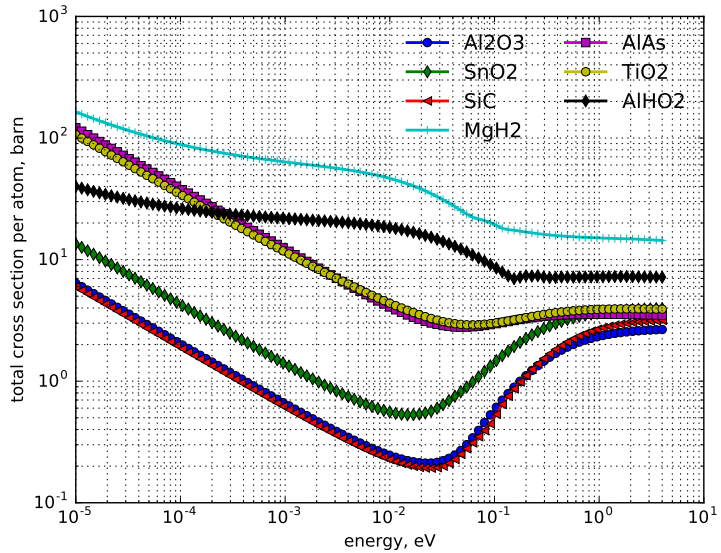

(h) MgF2

# Data mining is possible

## but how about the experimental validation?

Crystal atomic force constants can be calculated using DFT in a personal computer or obtained from databases, for example the **phonondb@kyoto-u** databased [5] made available by Dr. Atsushi Togo, which contains close to 600 crystalline materials. We show the room temperature cross sections of a few random materials that are produced based on the force constants in the database.




To validate the these cross sections, experimental data are needed.

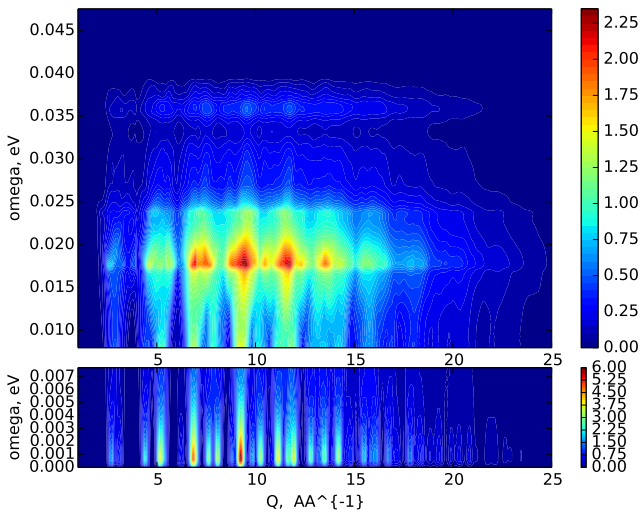
[5] http://phonondb.mtl.kyoto-u.ac.jp/database-mp.html

# Conclusion

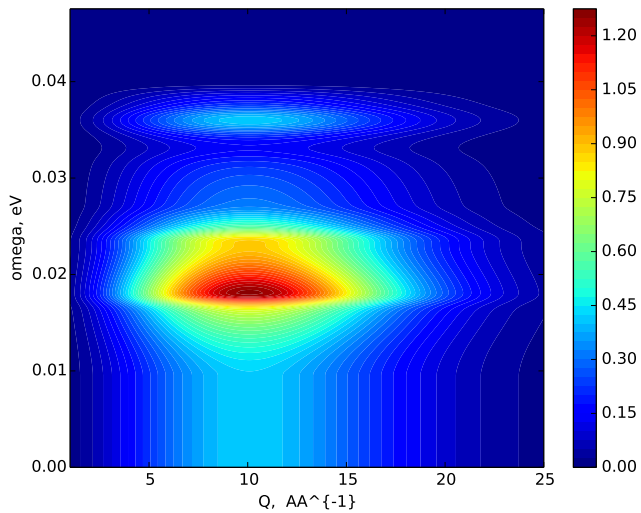
We conclude that the numerical implementation of our inelastic cross section model and final state sampler is accurate.

Also,

- Early access of NCrystal is possible by contacting us.
- A python-based package will also be released to enable users to launcher DFT calculations and generate NCrystal input file or coherent scattering kernel from a unit cell definition.




(a) coherent kernel




(b) incoherent approximation kernel