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SPALLATION
SOURCE

NJOY+NCrystal: Update of the Code and Thermal Scattering Library

2021 CSEWG Meeting

PRESENTED BY J.I. MARQUEZ DAMIAN

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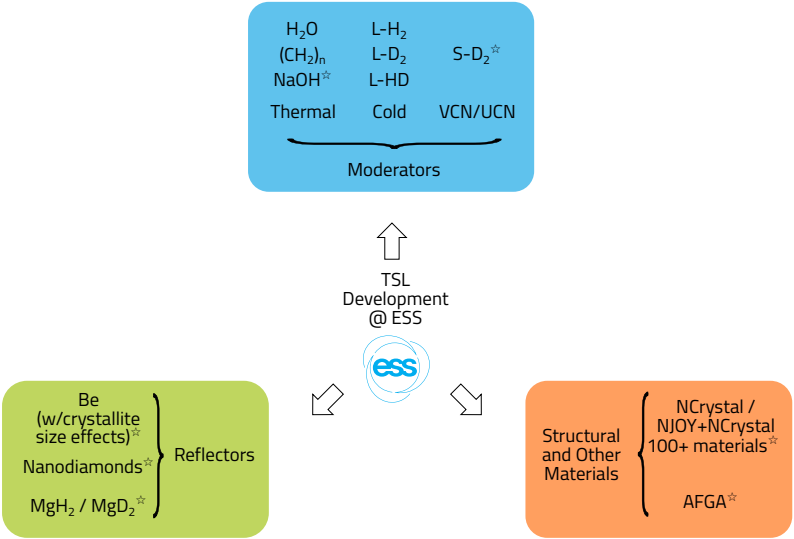
Acknowledgments

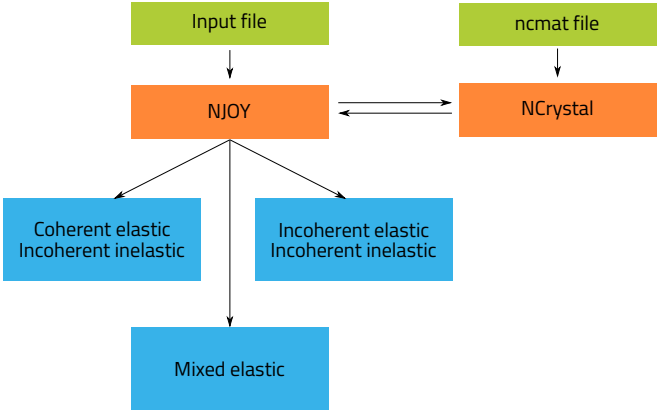
- To Xiao-Xiao Cai and Thomas Kittelmann for the development of NCrystal, which was used extensively in the work presented here.
- NJOY+NCrystal team: Kemal Ramic, Jose Ignacio Marquez Damian, Douglas D. Di Julio, Thomas Kittelmann, Davide Campi, Marco Bernasconi, and Valentina Santoro.
- To Atsushi Togo from Kyoto University and The Materials Project for providing extensive database of DFT phonon calculations.

This work was funded by HighNESS project at European Spallation Source ERIC under HORIZON 2020 grant agreement ID: 951782.



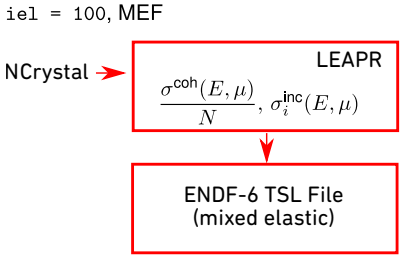
☆Developed using NCrystal

NJOY+NCrystal Workflow:



- Bragg edges ($E_{hkl} \cdot \sigma_{hkl}$), σ_b^{coh} and σ_b^{inc}, and σ_{free} are passed from NCrystal
- $S(\alpha, \beta)$ (the inelastic component) is calculated in LEAPR.

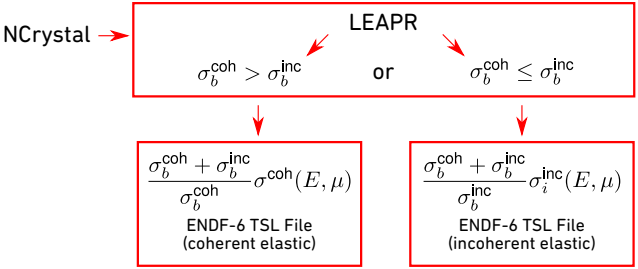
Description of elastic options



Simplified flow of NJOY+NCrystal when the mixed elastic option (MEF) is used.

Description of elastic options

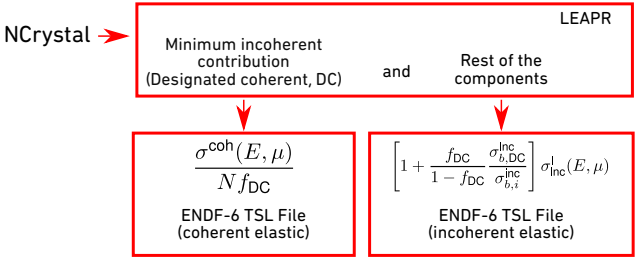
`iel = 99`, CEF (single atom case)



Simplified flow of NJOY+NCrystal when the curent elastic format (CEF) option is used for a monatomic scatterer.

Description of elastic options

`iel = 99`, CEF (molecule or compound)



Simplified flow of NJOY+NCrystal when the curent elastic format (CEF) option is used for a polyatomic or molecular scatterer.

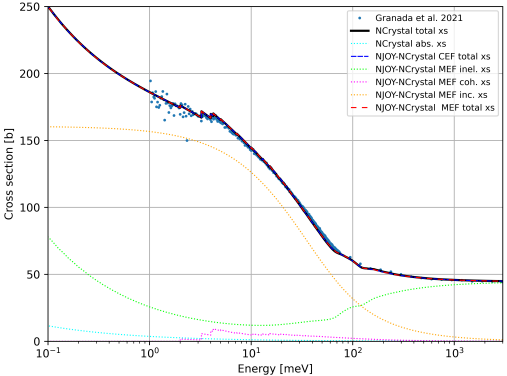
Inelastic/Elastic calculation consistency

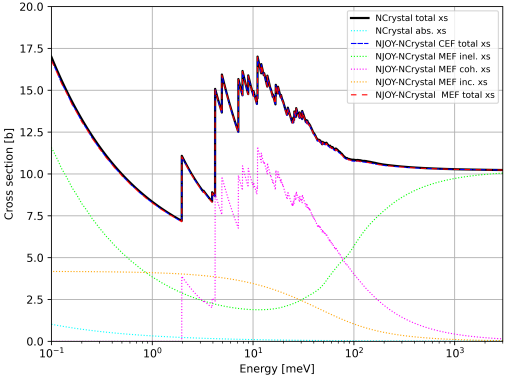
- LEAPR only handles the frequency spectrum of one component at a time, whereas NCrystal needs the Debye-Waller factor of all components to calculate the coherent elastic cross section.
- A consistency check is made using the *mean squared displacement* (MSD, $\langle u^2 \rangle$) value for each phonon spectrum. In NJOY+NCrystal we calculate $\langle u^2 \rangle$ using LEAPR and NCrystal, and write to the output file:

```
NCrystal MSD ........................  3.423E-03
LEAPR MSD ...........................  3.423E-03

doing temp =    -77.00

solid-type contributions to scattering law

frequency distribution
       e        rho(e)      beta     rho(beta)          bigp      t1(beta)
 0.00000    0.0000E+00    0.0000    0.0000E+00    1.2133E-02    3.5168E-02
```

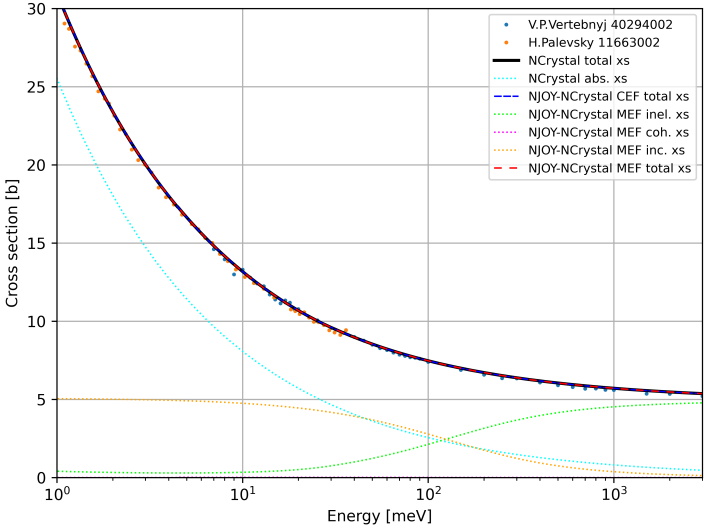
Of 2523 test calculations for 213 evaluations, 2224 (88%) have a difference below 0.1%, and all of them below 0.9%.

MgH_2 and MgD_2 as reflectors for HighNESS

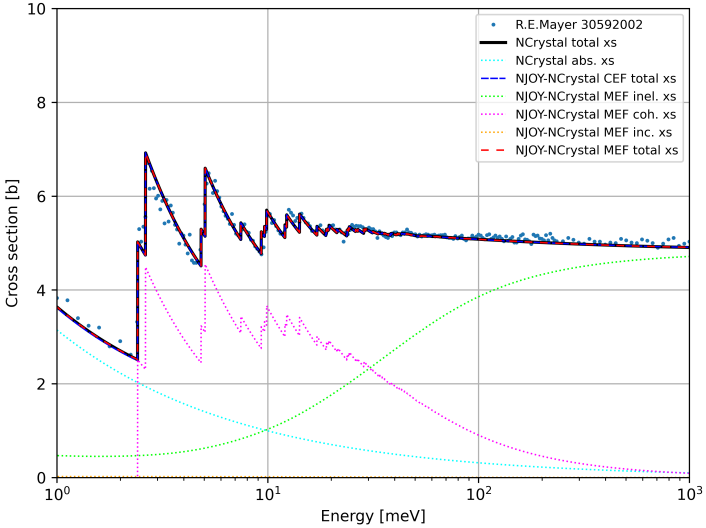




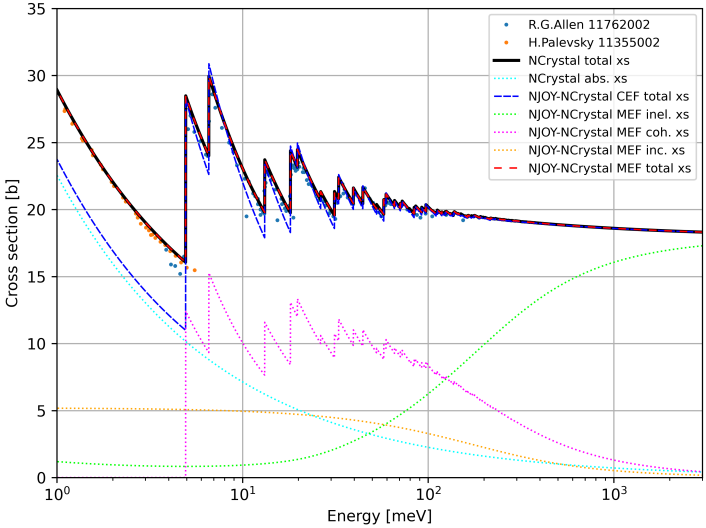
Vanadium (incoherent scatterer)



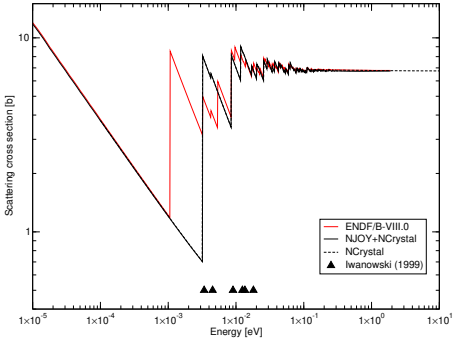
Tin (coherent scatterer)

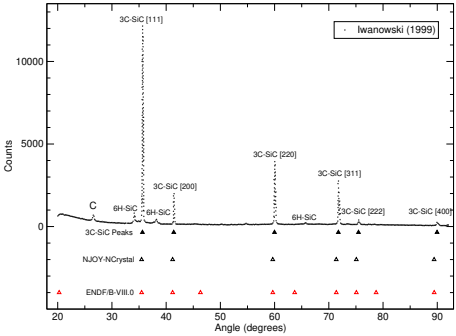


Nickel (mixed scatterer)



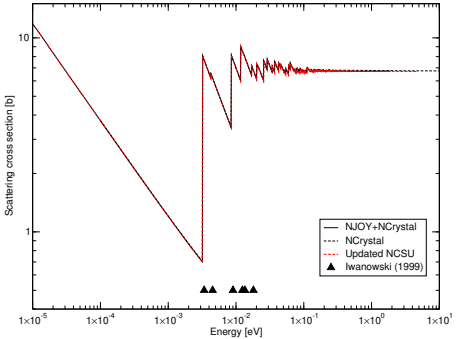
Validation: X-ray diffraction

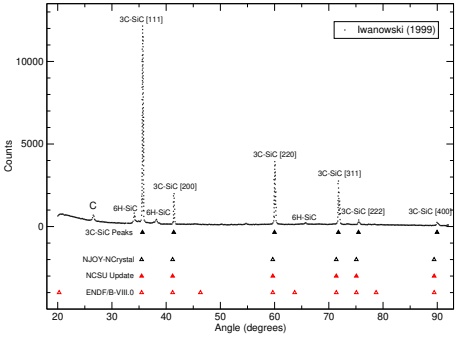




Comparison of total scattering XS (left) and X-ray diffraction (right) between NJOY-NCrystal and ENDF/B-VIII.0 for 3C-SiC (β-SiC).

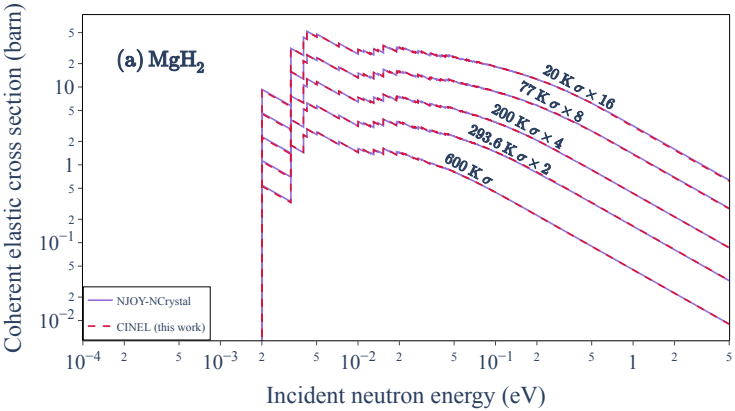
Validation: X-ray diffraction





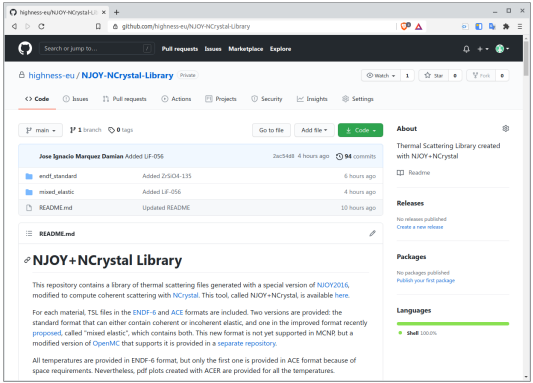
Comparison of total scattering XS (left) and X-ray diffraction (right) between NJOY-NCrystal and the updated NCSU evaluation for 3C-SiC (β-SiC).

Cross-comparison with CINEL



Comparison of calculations with NJOY+NCrystal and CINEL of the coherent scattering component in MgH_2. Thanks to Shuqi Xu from CEA-Cadarache.

Additional libraries



- Available online:
  `https://github.com/highness-eu/NJOY-NCrystal-Library/tree/v1.3`
- Version 1.3 includes adaptive alpha and beta grid, improved approximation for current ENDF format, and corrections after benchmarking with CINEL.

tsl-Ag
tsl-Al(Na4Si3Al3O12Cl)
tsl-Be(Be3N2)
tsl-Br(NaBr)
tsl-C(PbCO3)
tsl-Ca(CaO)
tsl-Cu
tsl-F(KF)
tsl-F(ZrF4-beta)
tsl-Ge(GeTe)
tsl-H(NaMgH3)
tsl-K(KF)
tsl-Li(LiH)
tsl-Mg(MgD2)
tsl-N(GaN)
tsl-Na(NaF)
tsl-O(Al2O3)
tsl-O(CeO2)
tsl-O(Li2O)
tsl-O(NaOH)
tsl-O(SiLu2O5)
tsl-O(TiO2-rutile)
tsl-O(ZrO2-tet)
tsl-Pb(PbO-alpha)
tsl-S(ZnS-sphalerite)
tsl-Si(SiC-beta)
tsl-Sn
tsl-Th(ThSiO4)
tsl-V
tsl-Zn
tsl-Zr(ZrO2)

tsl-Ag(AgBr)
tsl-Al(Y3Al5O12)
tsl-Bi
tsl-Br(TlBr)
tsl-C(SiC-alpha)
tsl-Ca(CaOH2)
tsl-Cu(Cu2O)
tsl-F(LiF)
tsl-Fe(Fe-alpha)
tsl-H(CaH2)
tsl-H(NaOH)
tsl-K(KOH)
tsl-Lu(Lu2O3)
tsl-Mg(MgH2)
tsl-N(Li3N)
tsl-Na(NaI)
tsl-O(BaO)
tsl-O(Cu2O)
tsl-O(Lu2O3)
tsl-O(Nd2O3)
tsl-O(SiO2-alpha)
tsl-O(Tm2O3)
tsl-O(ZrSiO4)
tsl-Pb(PbO-beta)
tsl-Sc
tsl-Si(SiLu2O5)
tsl-Sr
tsl-Ti
tsl-W
tsl-Zn(ZnF2)
tsl-Zr(ZrO2-tet)

tsl-Al
tsl-Al(YAlO3)
tsl-Bi(Bi2O3-beta)
tsl-C(Al4C3)
tsl-C(SiC-beta)
tsl-Ca(CaZrO3)
tsl-D(MgD2)
tsl-F(NaF)
tsl-Fe(Fe-gamma)
tsl-H(CaOH2)
tsl-H(SrH2)
tsl-La(La2O3)
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tsl-Mg(MgOH2)
tsl-N(Th3N4)
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tsl-O(Bi2O3-beta)
tsl-O(Dy2O3)
tsl-O(Mg2SiO4)
tsl-O(P2O5)
tsl-O(SiO2-beta)
tsl-O(Y2O3)
tsl-P(P2O5)
tsl-Pb(PbS)
tsl-Se(GaSe)
tsl-Si(SiO2-alpha)
tsl-Sr(SrF2)
tsl-Ti(TiO2-anatase)
tsl-Y
tsl-Zn(ZnO)
tsl-Zr(ZrSiO4)

tsl-Al(Al2O3)
tsl-Au
tsl-Bi(Ge3Bi4O12)
tsl-C(C-diamond)
tsl-Ca
tsl-Ce(CeO2)
tsl-Dy(Dy2O3)
tsl-F(PbF2)
tsl-Ga(GaN)
tsl-H(KOH)
tsl-Ho(Ho2O3)
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tsl-Mg
tsl-Mg(NaMgH3)
tsl-Na
tsl-Na(NaOH)
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tsl-Pb
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tsl-Al(Al4C3)
tsl-Ba
tsl-Br(AgBr)
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tsl-Cl(Na4Si3Al3O12Cl)
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tsl-I(NaI)
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tsl-Mg(Mg2SiO4)
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tsl-O(Ho2O3)
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tsl-O(PbCO3)
tsl-O(ThO2)
tsl-O(YAlO3)
tsl-Pb(Pb3O4)
tsl-Pt
tsl-Si(Mg2SiO4)
tsl-Si(SiY2O5)
tsl-Te(GeTe)
tsl-Tl(TlBr)
tsl-Y(Y2O3)
tsl-Zr

tsl-Al(AlN)
tsl-Ba(BaF2)
tsl-Br(KBr)
tsl-C(CaCO3)
tsl-Ca(CaF2)
tsl-Cl(NaCl)
tsl-F(CF4-alpha)
tsl-F(UF6)
tsl-Ge
tsl-H(MgH2)
tsl-K
tsl-Li(Li3N)
tsl-Mg(MgAl2O4)
tsl-N(AlN)
tsl-Na(NaBr)
tsl-Nd(Nd2O3)
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tsl-Th(ThO2)
tsl-U(UF6)
tsl-Y(YAlO3)
tsl-Zr(ZrF4-beta)

https://github.com/highness-eu/NJOY-NCrystal-Library/tree/v1.3

Conclusions

- NJOY+NCrystal is a user friendly, open source tool for the generation of TSL libraries for ordered materials.
- This tool was used to generate 200+ evaluations for 100+ new and updated materials, validated against total cross sections, specific heat capacity (C_p) measurements, and X-ray diffraction.
- From the first release back in May there were significant improvements in the code and the library.
- This improvement was benefited from cross comparison with different codes and libraries.

Thanks for your time.
Questions?