

McStas sample model functionality-matrix

(Master version available at the URL <https://confluence.esss.lu.se/display/MCSTAS/McStas+sample+model+functionality-matrix>)

Status of the McStas sample components, relevant for McStas 2.7 and 3.0 (Released December 2020)

	McStas sample comp + author info in italic	Model description	Main use areas	Incoherent scattering	Absorption	Bragg or other elastic scattering (type)	Inelastic scattering (type)	Multiple scattering	Non-trivial sample geometry
1	Incoherent (Vanadium, Plexiglass etc.) <i>McStas team</i>	Simple incoherent scatterer	Generic, imaging	✓	✓	✗	✗	✓	✓
2	Tunnelling_sample <i>McStas team / Kim Lefmann</i>	Idem 1, plus tunneling peaks and QE broadening	Quasi-elastic scattering, backscattering	✓	✓	✗	✗ ✓ (Quasi-elastic broadening + tunnel peaks)	✓ analytic approach)	✓
3	PowderN <i>McStas team / Peter Willendrup</i>	Debye-scherrer cones, tabular input (lau / laz)	Powder diffraction , imaging	✓	✓	✓ (Debye-Scherrer cones)	✗	✗	✓
4	Sample_nxs <i>Mirko Boin, HZB</i>	Debye-scherrer cones, unit-cell / atom input list	Powder diffraction , (future: imaging)	✓	✓	✓ (Debye-Scherrer cones)	✗ ✓	✓	✗
5	Single_crystal <i>McStas team</i>	Bragg spots, tabular input (lau). "Perfect imperfect" single crystal with mosaicity / lattice variation	Single crystal and MX diffraction	✓	✓	✓ (Bragg spots)	✗	✓	✓
6	Sans_spheres (and other similar) <i>McStas team and Martin Cramer Pedersen, KU</i>	Hard spheres in thin solution and other models, defined per-component...	SANS	✓	✓	✓ - SANS	✗	✗	✗
7	SANS_benchmark2 (and a few other stand-alone models) <i>Heinrich Frielinghaus, FZJ/JCNS</i>	Experimentally-benchmarked model set for SANS	SANS	✓	✓	✓ - SANS	✗	✓ up to 10 orders	✗
8	SASview_models <i>McStas team</i>	"Any" model from SASview / SASmodels	SANS	✓	✓	✓ - SANS	✗	✗ at this point	✗
9	Multilayer_sample <i>Rob Dalgliesh, ISIS STFC</i>	Multilayer-sample (additions of phase via matrix-formalism) with incoherent background	Reflectometry	✓	✓	✓ - Reflectivity curve	✗	✗	✗
10	Phonon_simple <i>McStas team / Kim Lefmann</i>	Single-branch acoustic phonon in FCC lattice	Inelastic scattering phonons	✗	✗	✗	✓ (phonon, at this point FCC lattice only)	✗	✗

11	Magnon_bcc <i>McStas team / Kim Lefmann</i>	BCC crystal n.n. and n.n.n. interactions only Can do either FM or AFM order upon a flag	Inelastic scattering FM/AFM magnons	✗	✗	✗	✓ (magnon, at this point BCC lattice only)	✗	✗
12	Isotropic_Sqw <i>McStas team / Emmanuel Farhi</i>	Structure and dynamics in isotropic materials (liquids, powders etc.)	Inelastic scattering, diffraction, isotropic materials, imaging	✓	✓	✓ (Debye-Scherrer cones)	✓ isotropic inelastic scattering	✓	✓
13	Res_sample <i>McStas team</i>	Resolution-oriented sample component	Generic	✓	✗	✗	✓ "flat, isotropic inelastic scattering"	✗	✗
14	TOFRes_sample <i>McStas team / Kim Lefmann</i>	Idem Res_sample, with TOF support	Generic	✓	✗	✗	✓ "flat, isotropic inelastic scattering"	✗	✗
15	Spot_sample <i>Garrett Granroth, SNS /ORNL</i>	Resolution-oriented sample component Dirac delta-functions in (Q and energy)	Inelastic scattering	✗	✗	✓	✓	✗	✗
16	Union components , <i>Mads Bertelsen, ESS</i>	A set of components that allows to build a complex sample/sample environment from basic geometries and physics/material properties	Generic	✓	✓	✓ Single crystalline or Powder crystalline	✓ - single acoustic phonon being included (2018)	✓	✓ - if built from cylinders, spheres, boxes, ...)
17	Single_crystal_inelastic <i>Duc Le, ISIS STFC</i>	4D-equivalent of Isotropic_Sqw / Single_crystal	Elastic and inelastic experiments with crystals	✓	✓	✓	✓	✓	?_?
18	Magnon_bcc <i>McStas team / Kim Lefmann</i>	FM / AFM magnon in BCC lattice	Inelastic scattering magnon	✗	✗	✗	✓ (magnon, at this point BCC lattice only)	✗	✗
19	NCrystal_sample <i>Xiao Xiao Cai, DTU Nutech /ESS</i>	Single crystal and powder diffraction, with isotropic inelastic scattering	Powder and Single_crystal diffraction, imaging	✓	✓	✓	✓ (in an isotropic form)	✓	
20	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo
21	"Polycrystal" <i>Alberto Cereser + Erik Knudsen, DTU Physics</i>	Engineering-diffraction / imaging oriented multigrain sample	Engineering-diffraction / imaging	✓	✓	✓ (Bragg spots)	✗	✓	✓
22	"Magnetic single crystal" <i>Linda Udby KU, + Erik Knudsen, DTU</i>	Bragg spots from lattice ala Single_crystal plus magnetic lattice. Tabular input (lau)	Single crystal magnetic diffraction	✓	✓	✓ (Bragg spots)	✗	✓	✓ / ?_?
23	"Specular reflectometry"	Use a reflectivity-curve with e.g. Mirror.comp	Reflectometry	✓	✓	✓ - Reflectivity curve	✗	✗	✗