System Requirements for MAGiC

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1 Introduction

1-1 Purpose of the document

This document describes the functional requirements for the subsystems of the Polarized Single Crystal Diffractometer for Magnetism. These requirements are based on the high level scientific requirements derived from the scientific case of the instrument as outlined in the instrument proposal as well as the Concept of Operations (ConOps) document that describes the expected operational use of the instrument. The subsystem requirements in this document are based on the conceptual design presented in the instrument proposal.

1-2 Definitions, acronyms and abbreviations

Each requirement is expressed as a natural language statement following the guidelines in the NASA Systems Engineering Handbook. Statements using the word “shall” express a strict requirement that has to be fulfilled for the system to be functional at all. Statements using the word “should” express a design objective beyond which the system performance does not increase. The requirements of this type are subject to trade studies. It should be noted that in many cases the value given is practically impossible to achieve, in which case the statement is equivalent to maximising or minimising the quantity in question. Statements using the word “must” express a capability that has to be achievable, but that is not part of the MAGiC work package scope. Any design or technical solution must not preclude these requirements to be fulfilled without significant rework.

1-3 References

1) MAGiC Concept of Operations document
2) NASA Systems Engineering Handbook, Washington, DC, USA: National Aeronautics and Space Administration (NASA). NASA/SP-2007-6105

2 System characteristics

2-1 System purpose

The instrument allows the collection datasets resulting from the scattering of polarized neutrons on single crystals.

2-2 System Overview

The instrument consists of three main technical subsystems: the beam transport and conditioning system (BTS), the sample exposure system (SES) and the scattering characterisation system (SCS). In addition the instrument includes the structures that house and support these subsystems and the software to control the instrument and process the data as described in the instrument product breakdown structure (PBS).

3. System requirements

High-level scientific requirements for the instrument (13.6.18)

1) The instrument shall provide a polarized incident beam over the $0.6<\lambda<6$Å wavelength range.
2) The instrument shall provide XYZ polarization analysis over 120°x6°.
3) The instrument shall allow data collection from crystals with a magnetic unit cell repeats of 100 Å.
4) The instrument shall allow data to be collected to a d_{min} of 0.35 Å.
5) The instrument shall match the size of the neutron beam to the size of the sample.
6) The instrument shall match the divergence of the neutron beam to the mosaicity of the sample.

7) The instrument shall allow data collection from crystals with volume lower than 0.001 mm^3
8) The instrument shall provide a cryogenic capabilities in the 30 mK - 300K range and magnetic field capabilities in the 0-10 T range.
9) The instrument should maximise the signal-to-background (S/B) ratio of the Bragg reflections.
10) The instrument should provide pulsed magnetic fields > 50 T.
11) MAGiC should serve the user and science and instrumental development program without interruptions during source operation
12) Instrument parameters that are defined as user selectable should be selectable with < 30 min delay.

3-1 Functional Requirements for MAGiC subsystems

3.1.1 Beam transport and conditioning system (BTS) (13.6.4.1)

Initial function statement
The "*beam transport system*" transports a beam of neutrons from the moderator surface to the sample. The size, divergence and wavelength spectrum of the beam are tailored to the needs of the experiment.

Functional requirements
1. Wavelength resolution

1.1. The BTS shall transport from the moderator a beam of neutrons to the sample at a distance that leads to a maximal wavelength uncertainty of 13% ($\Delta\lambda/\lambda$) for the detected neutrons using the full ESS pulse
1.2. Rationale: A moderate wavelength resolution allows the full pulse to be used while conserving the advantage of TOF for the S/B
1.3. Verification: Measurement of the longitudinal Q resolution on a reference sample

2. Beam size

2.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum size (full width half maximum) of 5.5 ± 0.5 mm and minimum size of 0.5 ± 0.1 mm.
2.2. Rationale: Matching the beam size to the sample size maximises the S/B
2.3. Verification: Measurement of the beam intensity profile at sample position

3. Beam divergence

3.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum divergence of ±0.3° and minimum divergence of ±0.1°.
3.2. Rationale: Matching the beam divergence to the sample mosaicity maximises the S/B
3.3. Verification: Measurement of the beam divergence at sample position

4. Beam size selection

4.1. The BTS shall transport from the moderator to the sample a beam of neutrons with a size selectable in 0.1 ± 0.05 mm steps.
4.2. Rationale: Matching the beam size to the sample size maximises the S/B
4.3. Verification: Measurement of the beam intensity profile at sample position

5. Beam divergence selection

5.1. The BTS shall transport from the moderator to the sample a beam of neutrons with a divergence selectable in 0.05° steps.
5.2. Rationale: Matching the beam divergence to the sample mosaicity maximises the S/B
5.3. Verification: Measurement of the beam divergence at sample position

6. Useful wavelength range

6.1. The BTS shall transport from the moderator to the sample a beam of neutrons with a bandwidth that lies within the wavelength range 0.6 ± 0.08 Å and 6.0 ± 0.08 Å.
6.2. Rationale: The selected wavelength band will define the Q-space covered by the instrument (number of reflections observed) and the resolvable unit cell size.
6.3. Verification: Measurement of the neutron spectrum at sample position

7. Incident beam polarization

7.1. The BTS shall transport to the sample a polarized beam of neutrons with a mean polarization rate of 97 % over the full accessible wavelength range.
7.2. Rationale : A high polarization rate maximize the instrument efficiency and the scientific throughput.
7.3. Verification : Measurement of the diffracted intensity for both spin states on a reference sample (FeCo, Heussler).

8. Incident spin flipping

8.1. The BTS shall flip the incident neutron spin state with an efficiency close to 100% over the whole wavelength range.
8.2. Rationale : Efficient spin-flip ensure conservation of the incident polarization rate.
8.3. Verification : Measurement of the diffracted intensity for both spin states on a reference sample (FeCo, Heussler)

9. Incident beam polarization axis

9.1. The BTS shall provide a way to align the polarization at sample position arbitrarily for neutrons of wavelength > 2 Å.
9.2. Rationale : XYZ polarization analysis allows separating the sample spin components.
9.3. Verification : Measurement of the diffracted intensity for x, y, z projection on a reference sample.

10. Scattered beam polarization analysis

10.1. The BTS shall provide analysis of the scattered neutrons spin state for neutrons of wavelength > 2 Å over a wide angle (120°x6°).
10.2. Rationale : polarization analysis is an unbeaten tool to separate magnetic and nuclear contributions to the diffraction pattern.
10.3. Verification : Measurement of the diffracted intensity for both spin states on a reference sample.

11. Beam focusing

11.1. The BTS should allow focusing of the beam over a 1x1 mm^2 area at sample position.
11.2. Rationale : Beam focusing increase neutron flux at sample position on micrometric samples.
11.3. Verification : Measurement of the neutron beam profile at sample position

12. Line-of-sight avoidance

12.1. When the experimental or optical cave is not interlocked the BTS shall block radiation from the target to a level required by safety regulations.

12.2. Rationale: The user must be able to change a sample
12.3. Verification: Measurement of the dose rate in the experimental cave

13. Brilliance transfer

13.1. The BTS should transport from the moderator to the sample a beam of neutrons with 100% brilliance transfer within the divergence range.
13.2. Rationale: Efficiency of the instrument will be linearly coupled to the BT
13.3. Verification: Measurement of the flux at sample position vs. flux at moderator surface

14. Divergence profile

14.1. The BTS should transport from the moderator to the sample a beam of neutrons with a maximum local deviation of 10% to a fitted Gaussian curve.
14.2. Rationale: The beam divergence profile is convoluted to the reflection profiles, which have to be smooth to allow integration by profile fitting
14.3. Verification: Measurement of the beam divergence profile at sample position

15. Wavelength selection

15.1. The BTS should transport from the moderator to the sample a beam of neutrons where the total brilliance outside the selected wavelength band is <1%
15.2. Rationale: The neutrons outside the used wavelength band add to the background
15.3. Verification: Measurement of the neutron spectrum at sample position

16. Accessibility

16.1. The BTS outside of the bunker should be accessible for repairs while the proton beam is on target.
16.2. Rationale: The instrument will be more fault tolerant hence increasing throughput of experiments
16.3. Verification: Measurement of the dose rate at the relevant technical component

17. Beamstop

17.1. The BTS shall absorb > 99.9 % of the neutrons not scattered by the sample
17.2. Rationale: The neutrons not scattered by the sample contribute to background and should not be incident on the detectors
17.3. Verification: Measurement with and without sample.

3.1.2 Sample exposure system (SES) (13.6.4.2)

Initial function statement

The sample exposure system positions the sample in a beam of neutrons and controls the physical and chemical environment of the sample as dictated by the needs of the experiment.

Functional requirements

1. Sphere of confusion

1.1. The SES shall maintain the position of the sample in the beam of neutrons with a sphere of confusion of ±0.02 mm root mean square for > 168 h.
1.2. Rationale: A sample of 0.1 mm dimension has to be homogeneously illuminated by the neutron beam during the entire experiment.
1.3. Verification: Optical imaging of the sample during sample rotation.

2. Sample rotation axis

2.1. The SES shall define the orientation of the sample in the beam of neutrons about a sample rotation axis that intersects the beam axis with a repeatability of ±0.02° within a range of 720°.
2.2. Rationale: The crystal orientation will be continuously changed during the experiment to cover the entire asymmetric unit in reciprocal space. The angular uncertainty should be small compared to the crystal mosaicity.
2.3. Verification: Optical imaging of a dummy object during sample rotation.

3. Sample rotation axis step

3.1. The SES shall change the orientation of the sample about the sample rotation axis in steps of 0.01°.
3.2. Rationale: The crystal orientation has to be changed during the experiment to cover the entire asymmetric unit in reciprocal space. The rotation should be quasicontinuous.
3.3. Verification: Optical imaging of a dummy object during sample rotation.

4. Continuous sample rotation

4.1. The SES shall continuously change the orientation of the sample about the sample rotation axis with angular speed in the $1 < w < 120$°/mn.
4.2. Rationale: A continuous sample rotation allows better extinction and absorption correction.
4.3. Verification: Optical imaging of a dummy object during sample rotation.

5. Rotation axis stability

5.1. The SES shall maintain the angle between the neutron beam axis and the sample rotation axis with a stability of 0.01°.
5.2. Rationale: The crystal orientation has to remain constant with respect to the neutron beam. The angular uncertainty should be lower than the typical crystal mosaicity
5.3. Verification: Optical imaging of a dummy object.

6. Sample temperature stability

6.1. The SES shall maintain the sample at a temperature of 0.05-300±0.1 K for > 168 h.
6.2. Rationale: The samples are very sensitive to temperature changes and need to be stabilised at ambient or cryogenic temperatures for the entire duration of the experiment.
6.3. Verification: Temperature measurement at sample position over extended time periods.

7. Sample magnetic field stability

7.1. The SES shall maintain the sample in a magnetic field of 0-10±0.02 T for > 168 h.
7.2. Rationale: The samples are very sensitive to magnetic field changes and need to be stabilised at zero or high field for the entire duration of the experiment.
7.3. Verification: Magnetic field monitoring over extended time periods.

8. Sample imaging

8.1. The SES shall allow optical imaging of the sample during the experiment.
8.2. Rationale: The sample has to be centered to the beam and rotation axis has to intersect the neutron beam axis.
8.3. Verification: Imaging a sample at the sample position.

9. Beam imaging

9.1. The SES shall allow optical imaging of the neutron beam at the sample position when a sample is not mounted.

9.2. Rationale: The sample has to be centered to the neutron beam and the rotation axis has to intersect the neutron beam axis (see ConOps).
9.3. Verification: Imaging the beam at the sample position.

10. Beam centroid determination

10.1. The SES shall allow the centroid of the neutron beam at the sample to be determined with an uncertainty of ±0.005 mm.
10.2. Rationale: The sample has to be illuminated by the neutron beam uniformly and hence the uncertainty in the beam centroid has to be smaller than the uncertainty in the sample position.
10.3. Verification: Repeated determination of the beam centroid.

11. Sample rotation axis orientation

11.1. The SES should be able to orient the sample rotation axis in an arbitrary angle to the neutron beam in the horizontal plane.
11.2. Rationale: Changing the orientation of the sample rotation axis allows a different set of reflections to be detected in a given direction allowing higher data completness. It also allows to perfectly match the crystallographic axis with the magnetic field main axis ensuring high quality data collection.
11.3. Verification: Test

3.1.3 Scattering characterisation system (SCS) (13.6.4.3)

Initial function statement

The scattering characterisation system detects the neutrons scattered by the sample to produce meaningful experimental data. It absorbs the neutrons that are not scattered into a beam stop.

Functional requirements

1. Detection efficiency

1.1. The SCS shall detect the scattered neutrons with an efficiency >45% across the whole wavelength band
1.2. Rationale: Neutron detection efficiency must be equivalent to current state-of-the-art technology.
1.3. Verification: Measurement of detection efficiency.

2. Spatial resolution

2.1. The SCS shall detect the scattered neutrons with a spatial resolution < 5 mm
2.2. Rationale: The spatial resolution allows resolving the reflections from a crystal with large magnetic unit cells. It should correspond at least to the expected diffraction spot size of 5 mm.
2.3. Verification: Imaging a reference grid.

3. TOF resolution

3.1. The SCS shall detect the scattered neutrons with a time-of-flight resolution < 0.02 ms
3.2. Rationale: The time-of-flight resolution should be an order of magnitude smaller than the minimal time width of a reflection, given by the shaped pulse length.
3.3. Verification: Measurement.

4. Neutron selectivity

4.1. The SCS shall detect radiation incident to the detector system other than thermal/cold neutrons with an efficiency <0.5%

4.2. Rationale: Non-neutron originated detector signals (e.g. gamma-rays) contribute to background and should be minimised
4.3. Verification: Measurement of detection efficiency for gamma-rays.

5. Accessible solid angle
5.1. The SCS shall be able to detect neutrons scattered by the sample within an horizontal angular range of ±170° and a vertical angular range of -18/+30° from the neutron beam axis.
5.2. Rationale: Detecting scattered neutrons at high diffusion angle increases the Q-space coverage of the instrument and therefore the amount of information collected.
5.3. Verification: Test

6. Detector stability
6.1. The SCS shall position the detectors with a stability of 0.1 mm.
6.2. Rationale: Vibrations or drift of the detectors should be small compared to the diffraction spot size
6.3. Verification: Survey and measurement of acceleration.

7. Neutron detection efficiency goal
7.1. The SCS should detect the scattered neutrons with an efficiency of 100% across the whole wavelength band.
7.2. Rationale: Neutron detection efficiency should exceed to current state-of-the-art technology.
7.3. Verification: Measurement of detection efficiency

8. Detection solid angle goal
8.1. The SCS should simultaneously detect the scattered neutrons within a solid angle of 4π sr.
8.2. Rationale: Detecting all scattered neutrons at once increases the amount of information collected in a given experimental time.
8.3. Verification: Test

9. Detector noise
9.1. The SCS should record <0.001 counts/s in the absence of incoming radiation.
9.2. Rationale: The lower the background the higher the achievable S/B ratio. The detector noise level must be lower than the background, otherwise the detector noise becomes limiting.
9.3. Verification: Measurement with shutter closed and the source not running

3.1.4 Experimental cave (13.6.4.5)

Functional requirements

The experimental cave houses the final beam defining elements of the BTS, the SES and the SCS. It shields the surrounding hall from the radiation generated by these systems as well as shielding the detector system from external radiation.

Initial function statement

1. Mounting components
1.1. The experimental cave shall allow the mounting of technical components of the BTS, SES and SCS with the required precision and stability
1.2. Rationale: The technical components have to be physically mounted on a suitable support.
1.3. Verification: Metrology and acceleration measurement

2. Utilities

2.1. The experimental cave shall provide the required utilities to the elements of the BTS, SES and SCS that are within it

2.2. Rationale: The technical components need utilities (power, cooling, vacuum, etc.).

2.3. Verification: Test

3. Access

3.1. The experimental cave shall allow access to personnel when the proton beam is on target

3.2. Rationale: Access for maintenance, repairs or adjustments is necessary.

3.3. Verification: Test

4. Biological shielding

4.1. The experimental cave shall shield its surroundings against the radiation produced by the neutron beam to safe levels according to ESS radiation safety regulations.

4.2. Rationale: The surroundings of the instrument must be safe for personnel

4.3. Verification: Dose rate measurement

5. Sample environment footprint

5.1. The experimental cave shall allow the mounting of sample environment devices < 800 mm in diameter and 1000 kg in weight.

5.2. Rationale: Extreme sample environments are large and heavy.

5.3. Verification: Test

6. Detector shielding

6.1. The experimental cave should shield the detectors from radiation to <0.001 neutrons/s.

6.2. Rationale: The lower the background the higher the achievable S/B ratio

6.3. Verification: Measurement with shutter closed

3.1.5 Control hutch

Initial function statement

The control hutch houses the experiment control and data processing terminals. During an experiment the user team spends most of their time in the control hutch.

Functional requirements

1. Instrument control terminal

1.1. The control hutch shall allow the user to remote control the technical components from a single dedicated computer terminal

1.2. Rationale: The instrument control should be possible from one terminal

1.3. Verification: Test

2. Data reduction terminal

2.1. The control hutch shall allow the user to process the neutron data to an indexed list of scaled reflections at a single dedicated computer terminal.

2.2. Rationale: Data reduction must be possible from one terminal during the experiment in order to verify data quality and perform preliminary data analysis.

2.3. Verification: Test

3. Comfort

3.1. The control hutch should be a comfortable working environment for the users

3.2. Rationale: Users work long hours and a comfortable environment reduces fatigue and increases productivity as well as safety.
3.3. Verification: User feedback

3.1.6 Hall 2

Functional requirements

The hall 2 contains all the shielding, infrastructure and support systems for the BTS elements within hall 2.

Initial function statement

1. Mounting components

1.1. The hall 2 shall allow the mounting of technical components of the BTS with the required precision and stability
1.2. Rationale: The technical components have to be physically mounted on a suitable support.
1.3. Verification: Metrology and acceleration measurement

2. Utilities

2.1. The hall 2 shall provide the required utilities to the elements of the BTS that are within it
2.2. Rationale: The technical components need utilities (power, cooling, vacuum, etc.).
2.3. Verification: Test

3. Access

3.1. The hall 2 should allow access to personnel when the proton beam is on target
3.2. Rationale: Access for maintenance, repairs or adjustments is necessary.
3.3. Verification: Test

4. Biological shielding

4.1. The hall two shall shield its surroundings against the radiation produced by the neutron beam to safe levels according to ESS radiation safety regulations.
4.2. Rationale: The surroundings of the instrument must be safe for personnel
4.3. Verification: Dose rate measurement

3.1.7 Hall 3 (13.6.4.9)

Initial function statement

The hall 3 contains all the infrastructure and support systems for the instrument components within hall 3.

Functional requirements

1. Mounting components

1.1. The hall 3 shall allow the construction of the optical and experimental caves with the required precision and stability
1.2. Rationale: The cave has to be built on a suitable support.
1.3. Verification: Metrology and acceleration measurement

2. Utilities

2.1. The hall 3 shall provide the required utilities to the optical and experimental caves.
2.2. Rationale: The technical components need utilities (power, cooling, gas, vacuum, etc.).
2.3. Verification: Test

3. Access

3.1. The hall 3 shall allow access to personnel when the proton beam is on target
3.2. Rationale: Access for maintenance, repairs or adjustments is necessary.
3.3. Verification: Test

3.1.8 Neutron guide hall (13.6.4.10)

Initial function statement

The neutron guide hall contains all the shielding, infrastructure and support systems for the BTS elements within the neutron guide hall.

Functional requirements

1. Mounting components

1.1. The neutron guide hall shall allow the mounting of technical components of the BTS with the required precision and stability
1.2. Rationale: The technical components have to be physically mounted on a suitable support.
1.3. Verification: Metrology and acceleration measurement

2. Utilities

2.1. The neutron guide hall shall provide the required utilities to the elements of the BTS that are within it
2.2. Rationale: The technical components need utilities (power, cooling, vacuum, etc.).
2.3. Verification: Test

3. Access

3.1. The neutron guide hall should allow access to personnel when the proton beam is on target
3.2. Rationale: Access for maintenance, repairs or adjustments is necessary.
3.3. Verification: Test

4. Biological shielding

4.1. The neutron guide hall shall shield its surroundings against the radiation produced by the neutron beam to safe levels according to ESS radiation safety regulations.
4.2. Rationale: The surroundings of the instrument must be safe for personnel
4.3. Verification: Dose rate measurement

3.1.9 Sample preparation area (13.6.4.11)

Initial function statement

The sample preparation area contains all the necessary equipment for sample handling, mounting and storage between experiments.

Functional requirements

1. Sample mounting

1.1. The sample preparation area shall allow the user to mount single crystals on any relevant mounting device.
1.2. Rationale: Crystals will have to be mounted for data collection.
1.3. Verification: Test

2. Sample storage

2.1. The sample preparation area shall allow storage of >500 single crystals at room temperature, in air, He or vacuum for >2 years.
2.2. Rationale: Crystals need to be safely stored before and after data collection.

2.3. Verification: Test

3.1.10 Integrated control and monitoring system (13.6.4.12)

Initial function statement

The integrated control and monitoring system allows the user to control the experimental parameters and process the neutron data. It also contains the control and monitoring systems needed for the safe operation of the instrument.

Functional requirements

1. Instrument control GUI

1.1. The integrated control and monitoring system shall allow the user to control the experimental parameters through a graphical user interface
1.2. Rationale: A good graphical user interface makes instrument control fast and easy
1.3. Verification: Test

2. Instrument control CLI

2.1. The integrated control and monitoring system shall allow the user to control the experimental parameters through a scriptable command line interface
2.2. Rationale: A good a scriptable command line interface allows for flexibility for more experienced users and ESS staff.
2.3. Verification: Test

3. Diffraction pattern visualisation

3.1. The integrated control and monitoring system shall allow the user to visualise the scattered neutron intensity as a function of detector coordinates and time-of-flight with user selectable binning.
3.2. Rationale: Visualisation of the diffraction pattern is crucial for judging the crystal and data quality. Generation of Laue-TOF or Laue diffraction patterns helps users familiar with single crystal diffraction.
3.3. Verification: Test

4. Data processing GUI

4.1. The Integrated control and monitoring system shall allow the user to process the recorded data through a graphical user interface to an indexed list of scaled reflection intensities
4.2. Rationale: A good graphical user interface makes data processing fast and easy.
4.3. Verification: Test

5. Data processing CLI

5.1. The Integrated control and monitoring system shall allow the user to process the recorded data through a scriptable command line interface to an indexed list of scaled reflection intensities
5.2. Rationale: A good scriptable command line interface allows for flexibility for more experienced users and ESS staff.
5.3. Verification: Test

6. Hazard detection

6.1. The Integrated control and monitoring system shall detect hazards that may compromise safety for personnel or equipment.
6.2. Rationale: Detection of hazards such as fire, radiation, flooding or asphyxiating gasses can prevent injury to personnel or damage to equpiment.

6.3. Verification: Test