Second Target Station (STS) Project: QIKR Requirements Document



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TBD

S04080100-SRD10000-R02

Second Target Station Project

QIKR REQUIREMENTS DOCUMENT

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Acronyms

FTS First Target Station

HVAC Heating, Ventilation, and Air Conditioning

IPPS Instrument Personnel Protection System

IRR Instrument Readiness Review

ODH Oxygen Deficiency Hazard

Q Wavevector Transfer (change in momentum of scattered neutrons)

RCRA Resource Conservation and Recovery Act

SiPM Scintillator Photo Multiplier

SCE Secondary Confinement Exhaust

STS Second Target Station

WBS Work Breakdown Structure

# Introduction

This document defines the functional requirements for the subsystems of the QIKR instrument. These requirements are based on the high level scientific requirements derived from science case outlined in the instrument proposal as well as those specified in the *S04010100-SR0001 Second Target Station (STS) Instrument Systems Requirements Document*. These requirements are supported by the *QIKR Technical Report*, S04080100-TRT10000.

# Scope

The project scope includes design, procurement, installation, testing without neutron beam, a Commissioning Plan and Fault Analysis, safety related operating procedures needed to perform commissioning (not user operation), technical support for document preparation (Hazards Analysis, Research Safety Summary, etc.) and completion of an Instrument Readiness Review (IRR).

The QIKR instrument consists of these major level 4 WBS groups:

* Optics
* Choppers
* Shielding
* Detectors
* Motion
* Sample Environment
* Infrastructure & Utilities

The QIKR instrument relies on additional WBS systems with requirements referenced here and defined by the documents indicated in the following sections:

* Section 11: Integrated Controls, WBS S.06.04.08
* Section 12: Scientific Software, WBS S.04.02

# Instrument Characteristics (S.04.08)

## Instrument Purpose

QIKR will be a general-purpose, horizontal-sample-surface reflectometer. Exploiting the increased brilliance of the Second Target Station (STS), QIKR will collect specular and off-specular reflectivity data faster than the best existing such machines. Utilizing pulse skipping (7.5 Hz), it will often be possible to collect complete specular reflectivity curves using a single instrument setting, enabling “cinematic” operation, wherein the user turns on the instrument and “films” the sample. Samples in time-dependent environments (e.g. temperature, electrochemical, magnetic, or undergoing chemical alteration) will be observed in real time with frame rates as fast as 1 Hz in favorable cases. Cinematic data acquisition promises to make time-dependent measurements routine, with time resolution specified during post-experiment data analysis. This capability will be deployed to observe such processes as *in situ* polymer diffusion, battery electrode charge-discharge cycles, magnetic and other hysteresis loops in real time, and membrane protein insertion into lipid layers.

## Instrument Overview

The range of scientific fields served by QIKR is large, requiring specialized sample environments to interrogate solid and free-liquid surfaces, as well as solid/liquid, liquid/liquid and solid/solid internal interfaces. Free liquid and liquid/liquid experiments (and to a lesser extent rheology) are constrained in that the sample surface is defined by gravity, and so cannot be tilted. The incident reflection angle in these cases must be defined by deflecting or sampling the angular divergence of the incident neutron beam. Free liquid surfaces and upper-subphase-transmitting liquid/liquid interfaces require a downward-directed incident beam, while lower-subphase-transmitting liquid/liquid interfaces and rheometers need an upward-directed incident beam. Solid and solid/liquid samples can be tilted and generally are not constrained by the incident-beam direction. Massive sample environments, such as cryogenic magnets, however, may also benefit from a non-tilted sample. Therefore, to address the interests of the entire scientific community, QIKR will feature both downward- and upward directed incident beams, each with its own sample table, detector, and associated beam conditioning.

Collecting data rapidly and accurately is important for all experiments, particularly ones involving kinetic measurements. True kinetic measurements would need to be collected at a single instrument setting covering the full *Q* range of interest. The 15-Hz STS repetition rate affords a much larger wavelength bandwidth than is available at the 60-Hz FTS, but to achieve true single-setting operation for most samples, QIKR will need to be able to run in frame-skipping mode at 7.5 Hz. Beyond rapid data acquisition, the neutron flux of the STS will enable experiments with unprecedented time resolution. In addition, while optimizing transport of short-wavelength neutrons at peak moderator flux (*λ* = 2.5 Å) is essential to maximize *Q* bandwidth and minimize counting time, the instrument will also be capable of operating at 15 Hz and in different wavelength bands. In such modes, one covers the full *Q* range with multiple incident beam settings.

As data acquisition time decreases, the proportion of time spent aligning samples or setting up and waiting for sample environments to equilibrate grows. To maximize time spent collecting data, time spent carrying out these support tasks should be minimized.

For further details, refer to the *QIKR Technical Report*, S04080100-TRT10000.

## High Level Instrument Requirements (S.04.08.01)

From the *Instrument Systems Requirements Document*, S04010100-SR0001, the following requirements are derived. The requirements in this table apply to both the upward- and downward-directed beamlines unless otherwise noted. Requirements throughout the remainder of this document refer back to these:

| Req. No. | Description | Traceability |
| --- | --- | --- |
| S.04.08.01-R1 | QIKR components shall be designed for a lifetime of at least 10 years | S.4-R03 |
| S.04.08.01-R2 | QIKR shall be designed to support ≥ 95% availability during beam operations*Note: Instrument equipment must be capable of operating throughout the 5000 hours of yearly planned STS facility operation.* | S.4-R04 |
| S.04.08.01-R3 | QIKR shall be capable of operating independently and without negatively impacting the performance of other instruments | S.4-R05 |
| S.04.08.01-R4 | QIKR equipment, including shielding, shall be designed to be removable/ replaceable and must use minimal amounts of RCRA-listed materials and materials that activate with long-lived isotopes | S.4-R06 |
| S.04.08.01-R5 | QIKR shall be capable of remote operations | S.4-R07 |
| S.04.08.01-R6 | QIKR shall be designed to operate safely and efficiently within the context of the user program | S.4-R08 |
| S.04.08.01-R7 | QIKR shall be designed to accept pulses from the STS moderator designed to support a downward-directed neutron beam | S.4-R09 |
| S.04.08.01-R8 | QIKR must be able to provide and maintain the level of optical component alignment required to meet the instrument’s performance goals over the lifetime of the instrument*Note: This may mean providing monitoring of alignment over time and ensuring it will be possible to perform realignment if needed* | S.4-R14 |
| S.04.08.01-R9 | QIKR equipment shall be designed following all applicable standards for personnel safety.*Note: Safety hazards will be evaluated within the framework of a formal hazards analysis identifying consequences, likelihood and proposed mitigation of hazardous events* | S.4-15 |
| S.04.08.01-R10 | QIKR shall be designed to limit radiation exposure in adjacent areas that are accessible to personnel during beam-on and beam-off conditions to less than 0.25 mrem/hr | S.4-R16 |
| S.04.08.01-R11 | QIKR must provide accommodation for additional shielding to be added to achieve low background: <2 counts/minute “dark count” (shutter closed) and <5 counts/sec with the shutter open and detector not viewing the beam*Note: The requirement is only to provide the ability to add shielding after beam-on if the detector counts require it* | S.4-R01 |
| S.04.08.01-R12 | QIKR must provide two main incident beams, one viewing the moderator from above the horizon, and one from below. | S.4-R01S.4-R09S.4-R13 |
| S.04.08.01-R13 | QIKR must be able to operate each beam path independently of the other | S.4-R01S.4-R09S.4-R13 |
| S.04.08.01-R14 | QIKR must provide multiple incident angles on both solid and liquid samples | S.4-R01S.4-R09S.4-R13 |
| S.04.08.01-R15 | QIKR must provide user facilities and equipment sufficient to prepare samples containing liquids for testing and to safely collect experiment data | S.4-R08 |
| S.04.08.01-R16 | Personnel must have safe access to each end station within 30sec of closing the corresponding shutter*Note: This will be determined by material and shielding choices* | S.4-R04S.4-R08S.4-R15 |
| S.04.08.01-R17 | There must be at least 46cm (1.5 feet) of clear space to the side of the sample for user access on each of the upper and lower beam paths | S.4-R08 |
| ~~S.04.08.01-R18~~ | Deleted, Rev02 |  |
| S.04.08.01-R19 | QIKR sample stage must accommodate sample equipment that fit within a 60cm x 60cm x 200cm volume (Length x Width x Height)  | S.4-R01 |
| S.04.08.01-R20 | Horizontal beam footprint at sample = 5x10 mm to 25x75 mm | S.4-R01 |
| S.04.08.01-R21 | QIKR must accept 95% of the viewable neutron trajectories from the moderator at the spectrum peak (λ = 2.5 Å) | S.4-R01S.4-R09 |
| S.04.08.01-R22 | QIKR must be able to operate at both 15 and 7.5 Hz | S.4-R01S.4-R02 |
| S.04.08.01-R23 | Q-resolution 0.02 ≤ ΔQ /Q ≤ 0.07 | S.4-R01 |
| S.04.08.01-R24 | Min Bandwidth (lower path) Min Bandwidth (upper path)Δλ = 16.8 Å at 7.5 Hz Δλ = 14 Å at 7.5 HzΔλ = 8.4 Å at 15 Hz Δλ = 7.0 Å at 15 Hz | S.4-R01S.4-R02 |
| S.04.08.01-R25 | QIKR shall be optimized for a relative angular resolution of 0.025, but shall support resolutions as large as 0.07 | S.4-R01 |
| S.04.08.01-R26 | The nominal sample position must be 2m away from the end of the guide, measured along the guide centerline | S.4-R01S.4-R09 |
| S.04.08.01-R27 | The nominal detector position must be on a 2m radius centered on the nominal sample position | S.4-R01S.4-R09 |

# Optics (S.04.08.02)

The neutron guide system will be designed to have the highest transmission efficiency for neutrons of wavelengths > 2.5 Å and will completely reject wavelengths < 0.25 Å. The guide system will also provide a sufficient number of wave vector transfers at the sample to allow a variety of neutron incident angles without requiring tilting of the sample itself. Configuration and Quality Level of the Optics System is given in the S04080200-QAI10000 document.

| Req. No. | Description | Value/Error | Traceability(S.04.08.01) |
| --- | --- | --- | --- |
| S.04.08.02-R1 | The QIKR neutron guide system shall have a design vacuum level less than 5x10-3 torr. | R13, R21, R23, R24, R25 |
| ~~S.04.08.02-R2~~ | Deleted, Rev02 |  |
| S.04.08.02-R3 | The range of wave vector transfers (neutron incident angles) supplied at the sample position shall be: | 0.005-0.5 Å-1  | R13, R14 |
| S.04.08.02-R4 | Neutron attenuation by the slits shall be: | <10-5 at 1 Å | R13, R21, R23, R24, R25 |
| S.04.08.02-R5 | Alignment of optical components must be such that each beam path transmits 2.5Å -25Å neutrons from the moderator to the sample with an efficiency of: | >90% of the simulated neutron transport | R08, R13, R21, R23, R24, R25 |
| ~~S.04.08.02-R6~~ | Deleted, Rev02 |  |
| ~~S.04.08.02-R7~~ | Deleted, Rev02 |  |
| S.04.08.02-R8 | Variation in position between guide elements must be less than the following maximums (refer to figures 1-2):horizontal/vertical linear:longitudinal linear:angular about the longitudinal axis:angular about the x or y axis: | Δx, Δy < 20 μmΔz < 100 μmΔƟ < 2.0x(10)-3 radiansΔφ < 2.0x(10)-3 radians | R08, R13, R21, R23, R24, R25 |
| S.04.08.02-R9 | Variation in position between guide sections must be less than the following maximums (refer to figures 1-2):horizontal/vertical linear:longitudinal linear:angular about the longitudinal axis:angular about the x or y axis: | Δx, Δy < 50 μmΔz < 2 mmΔƟ < 2.0x(10)-3 radiansΔφ < 2.0x(10)-3 radians | R08, R13, R21, R23, R24, R25 |
| S.04.08.02-R10 | QIKR must supply a means to evacuate the guide that is separate from the central bunker vacuum supply | R2, R6 |
| S.04.08.02-R11 | QIKR must supply a means to back-fill evacuated guides with house nitrogen*Note: this can be through the same connection where local vacuum is supplied* | R2, R6 |
| S.04.08.02-R12 | A high-pass wavelength filter must be present to reject unwanted long wavelength neutrons from prior pulses.*Note: The frequency cutoff is variable and is adjusted by filter angular position. The cutoff depends on instrument operation rate (7.5Hz or 15Hz) and the settings required for a particular experiment.* | R22, R24 |



**Figure 1**: Description of guide elements and guide sections. Guide elements are individual pieces of guide glass. Guide sections are each a single housing that contains multiple guide elements. Alignment requirements are applied both between guide elements and between guide sections.



**Figure 2**: Description of misalignment types: (a) misalignment of centers of adjacent guide element ends or guide section ends, (b) rotational misalignment between adjacent guide elements or guide sections along the longitudinal axis of the downstream guide element or guide section, (c) variation in longitudinal distance between adjacent guide element (or guide section) end centers, and (d) rotational displacement of a guide element’s (or guide section’s) downstream end center from its nominal position.

# Choppers (S.04.08.03)

QIKR will have bandwidth choppers sufficient to pass the desired wavelength range for each beam path and to reject all other wavelengths to the highest degree possible. To allow frame skipping, each chopper will also be able to rotate at half the source frequency (7.5Hz).

| Req. No. | Description | Value/Error | Traceability(S.04.08.01) |
| --- | --- | --- | --- |
| S.04.08.03-R1 | Neutron choppers shall have an availability requirement ≥ 97% to be operating within specification during beam operations | R2, R13 |
| S.04.08.03-R2 | Choppers must be removable within 24 hours of beam shutdown | R2, R4, R13 |
| S.04.08.03-R3 | Chopper rotation frequency: | 15Hz, 7.5Hz | R13, R22 |
| S.04.08.03-R4 | Choppers must supply a variable angular aperture | R13, R24 |
| S.04.08.03-R5 | Attenuation of neutrons outside of the desired wavelength range of 2.5 -23.5 Å shall be: | <10-5 at 1 Å | R13, R21, R23, R24 |

# Shielding (S.04.08.04)

QIKR will need sufficient shielding to both ensure that background radiation at the sample and detector is minimal, that safe radiation levels are always maintained outside the cave, and that safe radiation levels are maintained within the cave when the shutter is closed. Additionally, shielding within the cave will allow either the upper or lower beam path to be in full operation while the other is being accessed by personnel. QIKR has no separate beam transport shielding section: the cave begins immediately at the outer surface of the bunker wall. Material and size requirements for the shielding will be determined by neutronic analysis.

| Req. No. | Description | Traceability(S.04.08.01) |
| --- | --- | --- |
| S.04.08.04-R1 | The beamline shielding blocks, cave walls, and beam stop shall limit radiation exposure to a level of less than 0.25mrem/hour | R6, R9, R10, R13 |
| S.04.08.04-R2 | There shall be sufficient shielding in the bunker to absorb line-of-sight neutrons prior to the cave | R10, R11, R13, R16 |
| S.04.08.04-R3 | All shielding within the bunker space, within the bunker wall penetration window, and within the cave must be removable | R4, R13 |
| S.04.08.04-R4 | The QIKR cave must provide shielding to allow personnel access to one beam path’s sample while the other beam path is operating | R10, R13, R16 |
| S.04.08.04-R5 | QIKR must have separate beam stops in the cave areas, one each for the upper and lower beam paths | R4, R10, R13, R16 |

# Detectors (S.04.08.05)

QIKR will need detectors with high spatial resolution and the ability to see reflections from the sample over a range of angles about both the vertical axis (diffuse reflections) and the horizontal axis transverse to the beam (specular-plane reflections).

| Req. No. | Description | Value/Error | Traceability(S.04.08.01) |
| --- | --- | --- | --- |
| S.04.08.05-R1 | QIKR detectors shall be capable of being grounded to a dedicated infrastructure for instrument system use | R09, R13 |
| S.04.08.05-R2 | Spatial pixel area shall be: | < 0.1 x 0.1 cm2 | R13, R20, R23, R24, R25 |
| S.04.08.05-R3 | Minimum detector area shall be: | 20 x 20 cm2 | R13, R20, R23, R24, R25 |
| S.04.08.05-R4 | Precision of time-of-flight detection shall be: | 10 μsec | R13, R20, R23, R24, R25 |
| S.04.08.05-R5 | Total instantaneous rate shall be:Time-average rate shall be:Maximum dead time at these rates must be <1% | >20,000/sec>10,000/sec | R13, R20, R23, R24, R25 |
| S.04.08.05-R6 | Detector efficiency shall be: | >60% @ 2.5 Å | R13, R20, R23, R24, R25 |
| S.04.08.05-R7 | Diffuse angular range (rotation about the vertical axis) shall be: | -1o < 2φ < 15o | R13, R20, R23, R24, R25 |
| S.04.08.05-R8 | Specular-plane angular range (rotation about the horizontal axis perpendicular to the beam path) shall be: | -15o < 2θ < 15o | R13, R20, R23, R24, R25 |

# Motion (S.04.08.06)

In this section, the z-axis is defined to be along the centerline of the beam between the end of the beam guide and the sample (downstream is positive), the x-axis is horizontal, and the y-axis is perpendicular to x and z (upward is positive). The axes follow a right-handed coordinate system sign convention.

QIKR will have fixed beam path directions but will be able to change the angle of neutrons incident on the sample by selecting various beam intensities exiting from the guide at discrete angles and positioning the sample to intersect one of those beams, and/or by changing the orientation of the sample. The motion axes downstream of the guide end will select the desired incident angles and provide the desired detection coverage while controlling beam divergence and shaping the beam footprint on the sample. They will also place the sample in a y-position that intersects one of several desired beam intensity angles. Either upstream or downstream of the guide end will be located a beam attenuator that allows to user to reduce the overall beam intensity in discrete increments

The Maintenance Shield for QIKR will be a custom version of the standard design since it must accommodate two separate beam paths. The customization will be limited to the range of motion, overall size of the shield, and the total number of shield positions. The overall design and method of operation will otherwise be the same as the standard maintenance shield.

Each beam path will have its own Shutter, located downstream of that path’s chopper. Each Shutter will be operated independently of the other so that the upper beamline may be operational while the lower beamline is accessible to personnel (and vice versa). A heavy shutter may be used, but since QIKR is a curved beamline, it may be possible to use a lighter style of shutter, such as a guillotine.

Additional Motion Requirement details are given in **S04080600-SRD10000**.

| Req. No. | Description | Value/Error | Traceability(S.04.08.01) |
| --- | --- | --- | --- |
| S.04.08.06-R1 | QIKR must provide three collimating apertures upstream of the sample that have remotely adjustable openings. | R5, R20, R23, R25 |
| S.04.08.06-R2 | The apertures upstream of the sample must be movable along the beam path direction.*Note: This motion may be either manual or motorized, preference for manual motion* | R5, R13, R19, R20, R25 |
| S.04.08.06-R3 | QIKR must be able to remotely and collectively rotate all collimating apertures about an *x* axis drawn through the center of the guide glass end. | R5, R13, R14 |
| S.04.08.06-R4 | QIKR must be able to remotely adjust the sample position about its nominal location in the *x*-*z* plane. | R5, R13, R19, R26, R27 |
| S.04.08.06-R5 | QIKR must be able to remotely adjust the *y* axis position of the sample about its nominal location.*Note: There are three nominal y-positions of the guide defined by the three highest intensity beams exiting the guide end* | R5, R13, R14, R19, R26, R27 |
| S.04.08.06-R6 | QIKR must be able to remotely adjust the angle of the sample about each of the *x* and *z* axes relative to a horizontal plane. | R5, R13, R14, R19 |
| S.04.08.06-R7 | QIKR must be able to remotely adjust the position of the detector about an *x* axis through the center of the nominal sample location.  | R5, R13, R14, R26, R27 |
| S.04.08.06-R8 | QIKR must be able to remotely adjust the position of the detector about a y-axis through the center of the nominal sample position. | R5, R13, R26, R27 |
| S.04.08.06-R9 | Maintenance shield must be based on the standard design and accommodate both upper and lower beam paths. | R3, R7, R10, R12, R13 |
| S.04.08.06-R10 | Each shutter must be based on the standard design and be placed such that personnel can access one cave while the other is operating. | R6, R9, R10, R12, R13, R16 |
| S.04.08.06-R11 | QIKR must provide the ability to remotely move multiple samples sequentially into and out of the sample position. | R5, R6, R13, R15 |
| S.04.08.06-R12 | Top level assemblies of motion components located within the cave must withstand additional loading beyond the loads generated by the assembly weight itself | R2, R6, R9 |
| S.04.08.06-R13 | The detector must have position adjustments independent of the sample position to allow for initial setup and alignment | R8 |
| S.04.08.06-R14 | Motion components and assemblies must be protected from accidental changes in their desired location | R8 |
| S.04.08.06-R15 | Motion components and assemblies within the cave must not permanently locate components within a given envelop about the nominal sample center position:*Note: This is meant to preserve clear space for sample environments. Motion components may be within this area for smaller sample environments but must be movable to accommodate larger sample environments.* | .35m below lowest y-pos.50m above highest y-pos.50m all other directions | R19 |
| S.04.08.06-R16 | All motion components as well as their associated cabling and control rack spaces must be located outside of the required clear space for the user next to the sample | R17 |
| S.04.08.06-R17 | A beam attenuator shall be provided that allows the user to reduce the overall beam intensity in multiple discrete increments*Note: A reduction in beam intensity may be to allow accurate measurements in some situations* | R23, R25 |
| S.04.08.06-R18 | The high-pass wavelength filter must have an adjustable linear position for initial alignment to the beam path, and an adjustable angular position to select the desired wavelength cut-off | R22, R24 |

# Sample Environment

Section deleted, R02. All Sample Environments moved out of Instruments’ scope.

# Infrastructure & Utilities (S.04.08.08)

QIKR will have the following infrastructure items in common with the majority of beamlines: a control hutch with furniture and workstation equipment, standard connections to building utilities (electrical power, water, HVAC, networking), SCE, IPPS and ODH equipment, smoke detectors, fire alarms, and sprinklers. Infrastructure and utility items that are unique to QIKR are listed in the table below:

| Req. No. | Description | Traceability(S.04.08.01) |
| --- | --- | --- |
| S.04.08.09-R1 | QIKR equipment must be able to interface to standard STS utility distribution systems | R6, R9, R13 |
| S.04.08.09-R2 | QIKR design shall make provisions for all required safety systems | R6, R9, R13 |
| S.04.08.09-R3 | QIKR must provide a sample prep area with storage for samples and sample prep materials. The prep area will also provide a water supply with a filtrations system, a sink with a drain for rinsing glassware, and a fume hood. | R13, R15 |
| S.04.08.09-R4 | QIKR must provide a means of moving guide sections, in-cave shielding, sample environments, and any other in-cave equipment weighing more than 25lbs into and out of the cave | R4, R6, R9, R13, R15 |
| S.04.08.09-R5 | QIKR must provide an in-cave location in each cave to store multiple samples | R5, R13, R15 |

# Integrated Controls/ Software (S.06.04.08)

Instrument Control Systems (ICS) shall meet the requirements in S06040200-SR0001, *Integrated Control Systems Instruments Control and Data Acquisition Requirements Document*.

# Scientific Software (S.04.02)

Scientific software includes development of robust data reduction, visualization, and analysis for STS instruments. Requirements for scientific software will be developed prior to CD2.