QIKR – Quite Intense Kinetics Reflectometer

QIKR will be a versatile multipurpose reflectometer featuring horizontal sample geometry and a broad "single-shot" Q-range for structural and kinetic studies of solid, solid/liquid, and free liquid surfaces and interfaces. QIKR will collect specular reflectivity data at a single (ϑ, $\Delta\lambda$) instrument setting over a full decade of Q (e.g. 0.02 $Å^{-1}$ < Q < 0.20 $Å^{-1}$). In addition to radically simplifying data collection and reduction, "one-shot" measurements eliminate the 60–90 s required to change chopper phases and move motors between Q bands on existing SNS reflectometers, enabling broad-Q specular reflectivity to be measured in seconds or less. This purely kinematical advantage, coupled with improved STS cold flux, can yield ×100 improvements in time resolution.

Science Drivers

Neutron reflectometry covers a broad spectrum of science involving the growth, self-assembly, structure, and interactions of a wide variety of thin film materials and impacts many core areas of polymer, chemical, biological, and materials science. Because the advanced thin film materials of the future will be increasingly complex, there is an urgent and ongoing need to develop high performance neutron reflectometers to elucidate their structures over length scales range from 1 nm to 1000 nm.

The challenges to be met in soft condensed matter and the life sciences are as wide ranging as the topics investigated. While the sensitivity of neutrons to structural features offers a significant advantage in many types of multicomponent system, the recent literature shows a clear trend toward following time-dependent processes. These processes include, but are not limited to:[1]

- Self-assembly of surfactants, polymers, and proteins at solid and liquid interfaces
- Rearrangement processes in thin films: polymer interdiffusion, inter-layer movement, lipid flip-flop, and annealing/drying/exchange/wetting processes in composite films such as those used in photovoltaic applications
- Encapsulation and release of components in plastics, polymer blends, drug delivery and implant materials, and chemical and biological sensors
- Switchable materials that undergo structural changes in response to external chemical, mechanical, electrical, or magnetic stimuli
- Surface reactions that involve changes in film structure or chemical composition; e.g., enzyme catalysis, oxidation or other film degradation reactions, receptor-ligand binding, drug-target interactions, surface functionalization, etc.

Science Requirements

Kinetic studies like those described above are infeasible with any of the current SNS first target station reflectometers because of the need to use multiple instrument settings to collect data over the necessary Q-range. Requirements for a kinetics reflectometer include:

1. The ability to measure a full decade in Q (e.g. from 0.02 $Å^{-1}$ < Q < 0.20 $Å^{-1}$) in a single instrument setting.
2. Sample sizes that range from 1 – 15 cm^2.
3. Option for polarized beam and polarization analysis.
4. Wet chemistry lab adjacent to the instrument to support sample preparation.
5. Fully integrated suite of sample environments including a Langmuir trough, environment chamber, potentiostat and others.

[1] H. Wacklin and A. Vickery. "ESS Instrument Construction Proposal–FREIA" (2014).

Technical Description

QIKR could be placed on the high intensity coupled moderator or possibly the wider viewed face (3 x 6 cm^2) of the high peak brightness coupled moderator. The sample position will be placed as close to the moderator as possible to maximize the Q-range sampled in a single frame, approximately 13.5 m. At a total flight path of 15 m to the detector, the instrument will reach a maximum wavelength of 26 Å in the first frame of operation. Q_{min} of 0.02 $Å^{-1}$ is reached with a beam incident on sample at an inclined angle of 2.37 deg. Reaching Q_{max} = 0.2 $Å^{-1}$ at this same angle requires 2.6 Å neutrons which are at the peak of the spectral distribution of the moderator. QIKR requires a 20×20 cm^2 detector with 1 mm pixel resolution capable of a sustained count rate of 0.5–1 M counts/s and a peak count rate of 5–10 M counts/s. As the entire reflectivity curve is captured in a single instrument setting, the detector must have a dynamic range of 10^7. The neutron guide will be curved or possibly will incorporate a multi-channel bender and may employ elliptical focusing in the horizontal direction. One bandwidth neutron chopper (or possibly two) will define the incident neutron wavelength band.

Key parameters of QIKR

Parameter	Description
Moderator	High-intensity coupled moderator
Beam Size	variable as large as 1.5×3 cm^2; illuminating flat samples from 1 – 15 cm^2
Moderator–sample distance	as short as 13.5 m
Sample–detector distance	1.5 m
Wavelength range	2.5 Å ≤ λ ≤ 26 Å
Resolution	$\Delta\lambda/\lambda$ <0.01
Detector	^{3}He 2-dimensional position-sensitive detector (if possible)