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Conceptual Design of a Synchrotron Beamline Dedicated to Ultrafast Time-Resolved Small-Angle X-Ray Scattering

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Abstract—The optical scheme of a synchrotron beamline for measuring small-angle X-ray scattering curves with high temporal resolution is developed as a part of constructing the 1–3 Fast Processes beamline of the SKIF 4+ generation synchrotron radiation facility. Such measurements are badly needed nowadays to study the dynamic processes that occur with carbon particles when high-energy materials explode and other technological problems.

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INTRODUCTION

Small-angle X-ray scattering (SAXS) is actively used at all major synchrotron radiation facilities. This technique is especially suitable for probing the internal mesostructure of materials and determining the sizes of their local inhomogeneities in density. Such problems often arise in contemporary physics, chemistry, biology, and materials science. Researchers have recently started to use SAXS to monitor fast dynamic processes in real time, in order to, e.g., visualize the detonation of high energy materials.

The 1–3 Fast Processes beamline of the SKIF synchrotron radiation facility now under construction consists of two end stations (Dynamic Processes and Plasma) positioned along the X-ray beam. Time-resolved SAXS is to be employed at the Dynamic Processes end station [1].

The 1–3 beamline is primarily intended for studying fast and ultrafast processes in characteristic timescales of ps to ms. This type of studies was pioneered by three institutions in Novosibirsk Akademgorodok (the Lavrentiev Institute of Hydrodynamics, the Budker Institute of Nuclear Physics, and the Institute of Solid State Chemistry and Mechanochemistry) and supervised by the Siberian Branch of the Russian Academy of Sciences [2–6].

The field of synchrotron studies of ultrafast processes has grown tremendously over the last decade. Shock waves generated by either gas guns or lasers have become objects of intense studies at synchrotron radiation sites in the United Kingdom, France, and Germany. Instrumentation and experimental protocols for such studies have matured considerably [7–12]. With the dedicated facility of the Dynamic Compression Sector at the Advanced Photon Source (United States), SAXS data with spatial resolution down to 1 μm can now be acquired for nanosecond time intervals [13, 14].

SCIENTIFIC TASKS

The 1–3 Fast Processes beamline is primarily dedicated to studying dynamic processes under conditions of explosion or shock wave impact, with emphasis on the behavior of engineering materials under such nonequilibrium external loads. High-fps X-ray videos will allow us to measure rates of transformations or density distributions directly during shock wave compression. The atomic structure of dynamically compressed materials will be studied via X-ray diffraction & scattering techniques (including SAXS).

Time-resolved SAXS was first used at the Siberian Synchrotron and Terahertz Radiation Centre (VEPP-3 storage ring) to study real-time dynamics of carbon condensation upon the detonation of high energy materials [2, 3]). The initial experimental time resolution was sufficient to count only an integral SAXS signal covering a fixed range of scattering angles. Instrumentation upgrades and the construction of an improved beamline on the VEPP-4 storage ring allowed reliable measurements of the angular distribution of the SAXS signal, shedding light on the temporal evolution of carbon particle sizes [15, 16].

Time-resolved SAXS has proven its utility in studying the synthesis of metal nanoparticle [17], the propagation of combustion in nanothermites [18], the detonation of nanostructured high-energy materials [19], and dusting [20].

SAXS with high temporal resolution is now a well-established experimental tool for probing fluctuations in the density of a given material at the nanoscale level in microsecond time intervals [2–6, 14–20]. Unfortunately, the VEPP-4 storage ring (a first generation source of synchrotron radiation) is far from optimal for meeting the challenges that time-resolved SAXS now faces. Specific shortcomings include the large size of the electron beam (which prevents the probing of density inhomogeneities larger than 70 nm), low X-ray beam intensity, and the long time interval of more than 124 nanoseconds between adjacent electron bunches.

Unprecedented advantages of the proposed new beamline design include (a) a tiny transverse synchrotron beam that extends the usable range of SAXS scattering angles to probe inhomogeneities as large as 3 μm, (b) a single-bunch mode that allows submicrosecond temporal resolution, and (c) the feasibility of dynamic experiments with a large-volume explosion chamber suitable for detonating loads equivalent to 2 kg of TNT. The last will increase the value of studies by pushing explosion experiments toward realistic scales of practical relevance [1].

X-RAY OPTICAL SCHEME OF THE BEAMLINE

The optimum X-ray photon energy is 20–40 keV, since the SAXS curves of large explosive loads with diameters of up to 40 mm (and more) will be measured. A superconducting wiggler inside a straight section 6 m long was chosen as the best insertion device for the new beamline. The wiggler's parameters are a period of 27 mm, a peak magnetic field of 2.8 T, and number $N = 74$ of periods. The main storage ring of the SKIF synchrotron radiation facility will operate at an electron kinetic energy of 3 GeV, providing a record low horizontal radiation emittance of 75 pm rad and allowing us to classify it as a member of the 4+ generation of synchrotron radiation sources. Figure 1 compares the spectral characteristics of the SKIF wiggler to those of the earlier experimental setup at the VEPP-4 storage ring [1].

Characteristic rates to be measured on the titular beamline are at the km/s level. The synchrotron radiation source is uniquely suited for studying such pro-

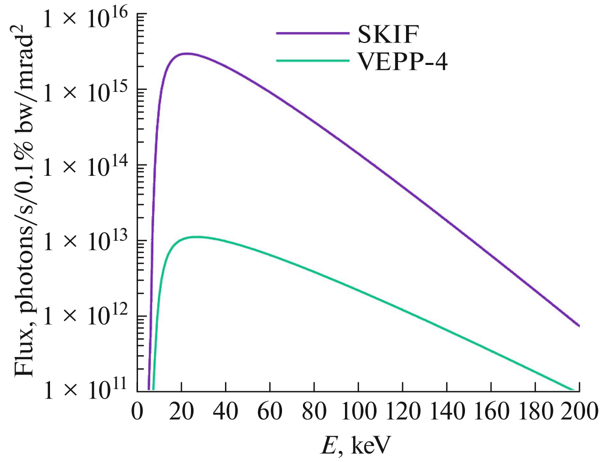

Fig. 1. Spectral characteristics of the source (allowing for attenuation of the beam in the front-end exit mirrors).

cesses because the duration of an X-ray pulse from a single electron bunch is ~3 ps, which determines the minimum required exposure time per detector frame. The apparent temporal resolution of a complete experiment (the delay between two detector frames) is determined by the time interval between two adjacent electron bunches/X-ray pulses, which can be tuned by selecting an appropriate pattern of bunch filling for the storage ring over a wide range of 3–100 ns. In contrast to other common synchrotron techniques, the charge of each electron bunch (rather than the nominal total electron current) is essential for time-resolved SAXS to acquire better experimental statistics [1]. Some critical TR-SAXS experiments could therefore require a special mode of storage ring operation with a specific pattern of bunch filling (i.e., a certain number of regularly spaced bunches) with the charge of each bunch maximized.

Note that it is better to use a wiggler as the source of radiation instead of the available types of undulators when employing the TR-SAXS technique. Typical undulators on a 3 GeV storage ring generate fundamental harmonics at 1.5–2.0 keV, but higher harmonics (11–17) unfortunately characterized by low intensity are needed to use hard X-rays at energies of 20 keV and above [1].

To monitor moderately fast (rather than ultrafast) processes with characteristic rates of no more than a few km/s, experimental statistics can be improved by integrating the signal over several consecutive electron bunches [1].

Using a pink rather than a monochromatic X-ray beam is another way of improving the attainable signal statistics at short periods of exposure. The feasibility of such an approach for obtaining interpretable SAXS curves has been demonstrated theoretically and experimentally [16, 21] for the total effective spectrum of the VEPP-4 facility (Fig. 1) . The quality of the SAXS

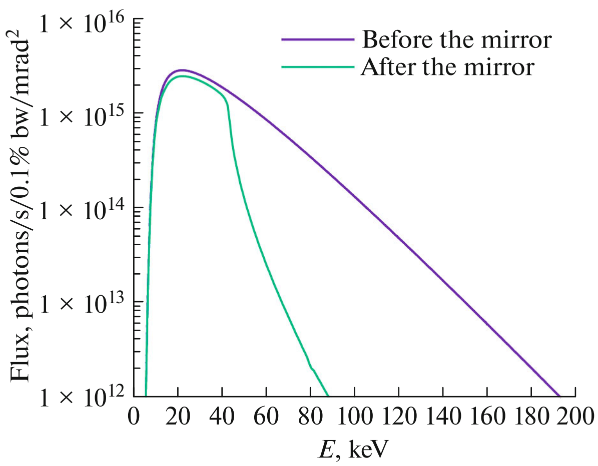

Fig. 2. X-ray spectrum before and after of the mirror.

data would nevertheless improve if highly intense X-ray pulses with narrow spreads of energy were available.

The soft X-ray component of the spectrum generated by the wiggler is attenuated by X-ray filters installed in both the front end and the X-ray beam transport pipeline. The front-end filter absorbs a considerable share of the thermal power, relieving the thermal stress on optical elements located downstream and improving on the stability of their operation.

An X-ray mirror is the next essential optical element of the beamline. It performs two functions simultaneously by focusing the X-ray beam at a distance of 120 m downstream and rejecting the high-energy component of the spectrum according to the short-wavelength threshold of external reflection (Fig. 2), in order to prevent distortion of the SAXS signal. A doubly focusing toroidal-shaped mirror was initially considered as such an element, but toroidal mirrors are expensive and hard to control. In the end, we chose a system of multi-sectional mirrors as a more cost-effective solution.

The radiation source is characterized by a very high total thermal power of ~36 kW. All optical elements, including the X-ray mirror, must therefore be cooled. A beam chopper or fast shutter located immediately after the front end is used to reduce both the radiation and the thermal loads on the elements located downstream. It should switch to the open position and let the beam pass through in only the short times required for an experiment (~100 μs–20 ms). The chopper is a set of solid metal discs, each of which has a narrow slit that rotates around a common axis at different rates. The X-ray beam can pass through the chopper only when all slits are aligned along the same plane. Otherwise, the radiation is absorbed by the discs.

An assortment of dedicated high-tech equipment will be used on the beamline to perform shock wave compression experiments. These components include two gas guns (calibers of 20 and 50 mm) and two explosion chambers (to detonate explosive loads equivalent to 200 and 2000 g of TNT). SAXS signals will be registered by a DIMEX silicon detector [22] and high-rate Nanogate cameras.

The general optical layout of the 1–3 Fast Processes beamline is shown in Fig. 3.

FUNCTIONAL ANALOGS

There are several installations in Russia and abroad that are dedicated to similar experiments. The number of such facilities has grown worldwide in recent years.

Studies of fast processes primarily associated with high-energy materials can be performed on the Submicrosecond Diagnostics and Extreme States of Matter beamlines at the Budker Institute of Nuclear Physics' Siberian Center of Synchrotron and Terahertz Radiation. The former beamline was launched in the late 1990s, while the latter was commissioned in 2014 [2–6]. The Dynamic Compression Sector facility

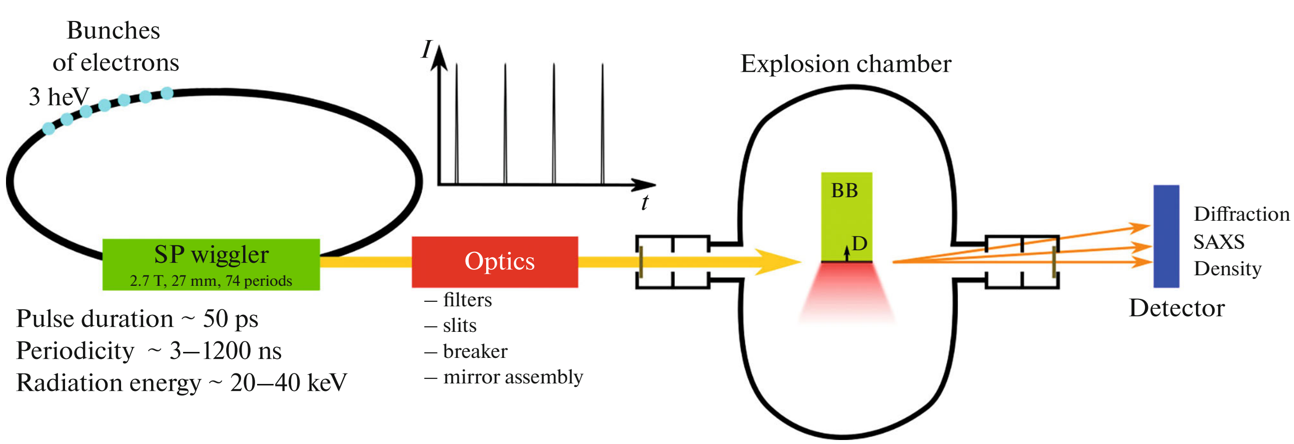

Fig. 3. General optical layout of the 1–3 Fast Processes beamline.

inaugurated in 2014 at the United States' Advanced Photon Source is the only one with similar functionality that can measure SAXS with temporal resolution comparable to those at international centers of synchrotron radiation [13, 14].

Analogous beamlines suitable for studying fast processes can be found at synchrotron sites in the United Kingdom, France, and Germany. These instruments do not specialize in studying high-energy materials, but they can provide useful information relevant to other types of fast processes [7–12].

CONCLUSIONS

A conceptual design was presented for the 1–3 Fast Processes beamline on the SKIF synchrotron radiation facility, which will be used to measure small-angle X-ray scattering curves with high temporal resolution.

It is planned to use a superconducting wiggler as the source of radiation for the beamline. A multi-section focusing mirror limits the photon spectrum at the position of a sample from the high-energy side.

Our design will allow us to reconstruct micro- and macroscopic properties of high energy materials on the beamline, contributing to the ongoing task of compiling equations of state for high-energy materials. New practical knowledge on the propagation of shock waves in engineering materials will be gathered with allowance for scaling effects. Fundamental patterns of detonation-related chemical reactions will be established, and innovative new ways of probing ultrafast processes will be developed.

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CONFLICT OF INTEREST

The authors declare they have no conflicts of interest.

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