Feasibility of Rapid and Sensitive XAFS Using Tunable X-Ray Undulators

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1. Introduction

We here propose several novel techniques to overcome the two problems, 1) the band width of undulator radiation is often narrower than the scanning range of ~1 keV usually required, and 2) the harmonics of radiation must cover the absorption edge energies. The proposed tunable X-ray undulator also provides a versatile means to optimize a brilliance to either XAFS or scattering experiments using variable band width capability. Quick scanning of monochromator has recently been used for a rapid measurement of XAFS [1]. Highest brilliance will be ideally achieved with a combination of fully independent tuning of undulator gap and synchronized scanning of monochromator. For an EXAFS measurement, however, this might impose a severe technical problem with both mechanical motion of undulator gap and beam stabilization. Although an X-ray undulator is a promising highly brilliant light source, two problems arise in XAFS experiments: 1) the band width of undulator radiation is often narrower than the scanning range of ~1 keV usually required, and 2) the harmonics of radiation must cover the absorption edge energies.

2. Conceptual Models

2.1 Q-scan I

Varying the deflection parameter K by changing a magnet gap, one can shift the fundamental and higher harmonic radiations. If there is a slight taper in the undulator gap, the harmonics will have broader maxima in the spectrum. In Fig. 1, the principle is schematically shown along with the energy scan method in EXAFS measurements, which will be referred to as quick (Q)-scan I [2].

A time resolution in Q-scan I is practically limited by either the maximum speed of the monochromator scanning or that of encoder reading. This kind of limitation does not appear in the energy-dispersive geometry, in which a cylindrically bent crystal focuses quasi-parallel white X-ray beam on the sample so that spectra are observed as a function of linear position behind the focus. For concentrated samples in a transmission mode, one can fully utilizes the polychromatic beam: the distribution of either an incident or a transmitted beam is obtained simultaneously.

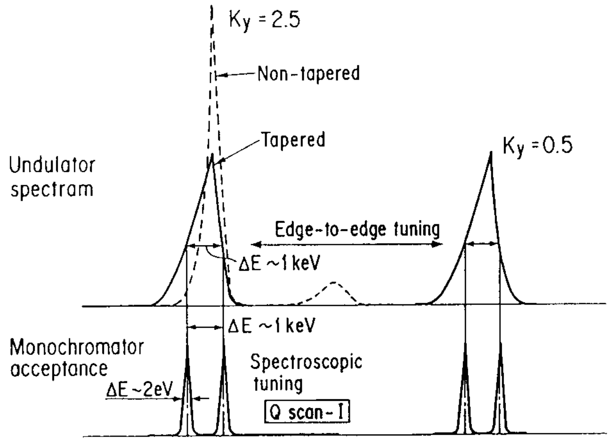

Fig. 1 Schematic of novel rapid XAFS technique, Q-scan I. Monochromator is rapidly scanned.

Presently, a time resolution in the order of 100 msec is obtained for concentrated samples in this geometry. Feasibility of time-resolved experiments of a transmission mode in the energy-dispersive geometry and highly brilliant beams was discussed elsewhere [3]. A major difference between the beamline setup of an undulator and that of a normal bending magnet is that a dispersing mirror is installed on the former. The dispersive geometry can not be applied to the fluorescence detection mode which requires a point-by-point data acquisition.

2.2 Q-scan II

On the other hand, an alternative quick-XAFS technique (hereafter referred to as Q-scan II) can be used with a variable bandwidth undulator [2]. Figure 2 shows a schematic for the technique, in which a polychromatic beam in an energy-dispersive geometry is spatially limited by a narrow slit. Quasi-monochromatic beam is rapidly scanned around the broadened fundamental or third harmonic radiation.

During the monochromator scan in a conventional setup, the undulator gap should be varied to covering about 1 keV energy width of XAFS measurement. Since the speed of synchronizing the undulator gap is limited in Q-scan I, we proposed the tapered undulator with a variable tilt angle. In this case, the tapered undulator gap can be fixed during the monochromator scan. Independent tuning for choosing an appropriate absorption edge can be completed within a definite time after the injection of electron/positron to a storage ring in order to minimize the disturbance. If an energy-dispersive geometry is used as a means of quick energy scan, a rapid and sensitive measurement can be achieved [4].

3. Summary and Discussion

Variable gap undulator can provide quasi-parallel X-ray beams to cover a wide range of energy by using the fundamental and third harmonics. For tuning to a particular absorption edge, an undulator gap is varied. Parallel setup of undulator magnet jaws is slightly tilted to introduce a taper to broaden a band width. For rapid and sensitive XAFS, a monochromator is scanned (Q-scan I) synchronizing the variation of the K-parameter or within a broadened undulator radiation. For further rapid or time-resolved studies, a new technique based on an energy-dispersive geometry is proposed (Q-scan II). These techniques can provide a means of rapid and sensitive XAFS for dilute systems. Further, the proposed undulators can be used for a microprobe XAFS with a high energy resolution which can map the distribution of both element and chemical state. Thus, the proposed technique will allow us to go beyond the present limitations with sensitivity and resolutions in time and space. Particularly, they will advance XAFS research of dilute systems such as surfaces, impurities, dilute alloys and biological systems. Since XAFS and crystallography are complementary techniques, it is desirable to design a beamline which can provide either a broad band width radiation or the maximum brilliance one depending on the purpose.

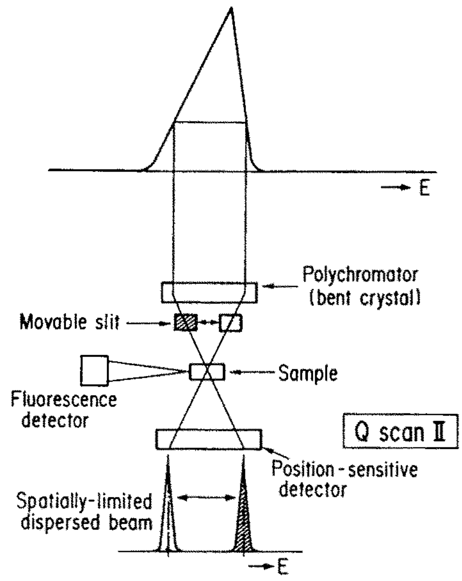

Fig. 2 Schematic of novel rapid XAFS technique Q-scan II. A slit is scanned in an energy-dispersive geometry.

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