Sirepo: a web-based interface for physical optics simulations – its deployment and use at NSLS-II

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ABSTRACT

"Sirepo" is an open source cloud-based software framework which provides a convenient and user-friendly web-interface for scientific codes such as Synchrotron Radiation Workshop (SRW) running on a local machine or a remote server side. SRW is a physical optics code allowing to simulate the synchrotron radiation from various insertion devices (undulators and wigglers) and bending magnets. Another feature of SRW is a support of high-accuracy simulation of fully- and partially-coherent radiation propagation through X-ray optical beamlines, facilitated by so-called "Virtual Beamline" module. In the present work, we will discuss the most important features of Sirepo/SRW interface with emphasis on their use for commissioning of beamlines and simulation of experiments at National Synchrotron Light Source II. In particular, "Flux through Finite Aperture" and "Intensity" reports, visualizing results of the corresponding SRW calculations, are being routinely used for commissioning of undulators and X-ray optical elements. Material properties of crystals, compound refractive lenses, and some other optical elements can be dynamically obtained for the desired photon energy from the databases publicly available at Argonne National Lab and at Lawrence Berkeley Lab. In collaboration with the Center for Functional Nanomaterials (CFN) of BNL, a library of samples for coherent scattering experiments has been implemented in SRW and the corresponding Sample optical element was added to Sirepo. Electron microscope images of artificially created nanoscale samples can be uploaded to Sirepo to simulate scattering patterns created by synchrotron radiation in different experimental schemes that can be realized at beamlines.

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Keywords: Sirepo, SRW, cloud computing, synchrotron radiation, NSLS-II

1. INTRODUCTION

We present a portable and user-friendly tool for scientific simulations named Sirepo. Our interface provides a convenient way to perform such portable simulations. Sirepo consists of a graphical web interface based on JavaScript with a backend server (either on local machine or a remote server) able to serve many different software packages, including already implemented interfaces with Synchrotron Radiation Workshop (SRW) for accurate X-ray source and optics simulations[1,2,3], Shadow3 – a ray optics code with many sophisticated features for X-ray beamlines[4,5], and a number of codes for particle accelerators simulations. The source code of Sirepo could be quickly extended[6] to support the codes from different scientific domains such as condensed matter physics, material science, chemistry, biology and other areas utilizing codes which require complex and at the same time flexible input and comprehensive output in the form of interactive visualization, data files and unified exchange format.

In the present work, we will focus on SRW, which is used at light source facilities for design and optimization of X-ray sources and beamlines by means of simulation of wavefront propagation through optical system of the X-ray beamlines. It is written in C++ with Python bindings. A "Virtual Beamline" module is used for convenient way to execute simulations in console. SRW is also interfaced with WaveMetrics' Igor Pro for advanced simulations, data analysis and visualization of the results. Sirepo is a complementary interface build on top of SRW-Python interface, allowing to perform comparable advanced simulations and data visualization in a browser. Below we will explain the implementation and main features of Sirepo and the details of the Source and Beamline pages. Finally, we will discuss basic examples and advanced simulations, including virtual beamlines implemented for NSLS-II.

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Simulation of experiments with partially-coherent X-rays using "Synchrotron Radiation Workshop"

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ABSTRACT

High-accuracy physical optics calculation methods used in the "Synchrotron Radiation Workshop" (SRW) allow for multiple applications of this code in different areas, covering development, commissioning, diagnostics and operation of X-ray instruments at light source facilities. This presentation focuses on the application of the SRW code for the simulation of experiments at these facilities. The most complete and most detailed simulation of experiments with SRW is possible in the area of elastic coherent scattering, where the interaction of radiation with samples can be described with the same transmission-type "propagators" that are used for the simulation of fully- and partially-coherent radiation propagation through X-ray optical elements of beamlines. A complete "source-to-detector" simulation of such an experiment for a lithographic sample is described here together with comparisons of the simulated coherent scattering data with actual measurements results, obtained at the Coherent Hard X-ray (CHX) beamline of the National Synchrotron Light Source II (NSLS-II). Particular attention is paid to the analysis of visibility of speckles and intensity levels in the scattered radiation patterns at different degrees of coherence of the radiation entering the sample.

Keywords: synchrotron radiation, X-rays, physical optics, partial coherence, coherent scattering, computer simulations

1. INTRODUCTION

Complete, "source-to-detector", simulations of experiments at light source facilities have a large number of benefits. Such simulations can allow for an accurate estimation of the feasibility of a given experiment, with a given sample, with a required resolution, at a particular beamline. This can be particularly important for new types of samples that are considered to be used in known types of experiments, and / or possibly for the development of new experimental schemes or even new types of experiments. The simulations can greatly help to determine optimal source and X-ray optics settings for a given experiment with a given sample (undulator gap and crystal angles, slit sizes, mirror radii of curvature, CRL configurations, etc.), determine optimal detector location, estimate expected radiation intensity distribution at the detector, required exposure time for a single measurement, duration of the entire experiment, etc. This can help to reduce the number of miscellaneous auxiliary measurements during experiment preparation and save expensive beam time. We note that such optimizations of beamline settings are particularly important for the experiments exploiting radiation coherence at modern storage ring based light sources, where, because of partial coherence of the generated radiation, a compromise between degree of radiation coherence (that typically determines resolution) and flux at the sample has usually to be done. Simulation of experiments can help to develop, test and tune experimental data processing algorithms, using simulated data, long before actual measurements. After the experiment, simulations can help to interpret the obtained experimental results more accurately. Simulations can also help to analyze impacts on quality of experimental data from miscellaneous electron beam and X-ray optics instabilities and other imperfections that may take place in a beamline, and to develop best strategies and priorities for their reduction or elimination.

Accurate simulation of emission and propagation of fully- and partially-coherent X-ray range Synchrotron Radiation (SR) through optical elements and drift spaces to a sample, using the SRW code [1] is currently done routinely for X-ray beamlines at NSLS-II [2] - [10]. The code uses Fourier optics and compatible methods for the simulation of fully-coherent radiation propagation, and it simulates partially-coherent radiation propagation through beamlines of storage-ring based SR sources by "summing-up" results of propagation of the fully-coherent radiation emitted by different "macro-electrons" seeded over the electron beam phase space [4].

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Main functions, recent updates and applications of "Synchrotron Radiation Workshop" code

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ABSTRACT

The paper presents an overview of the main functions and new application examples of the "Synchrotron Radiation Workshop" (SRW) code. SRW supports high-accuracy calculations of different types of synchrotron radiation, and simulations of propagation of fully-coherent radiation wavefronts, partially-coherent radiation from a finite-emittance electron beam of a storage ring source, and time-/frequency-dependent radiation pulses of a free-electron laser, through X-ray optical elements of a beamline. An extended library of physical-optics "propagators" for different types of reflective, refractive and diffractive X-ray optics with its typical imperfections, implemented in SRW, enable simulation of practically any X-ray beamline in a modern light source facility. The high accuracy of calculation methods used in SRW allows for multiple applications of this code, not only in the area of development of instruments and beamlines for new light source facilities, but also in areas such as electron beam diagnostics, commissioning and performance benchmarking of insertion devices and individual X-ray optical elements of beamlines. Applications of SRW in these areas, facilitating development and advanced commissioning of beamlines at the National Synchrotron Light Source II (NSLS-II), are described.

Keywords: synchrotron radiation, X-rays, insertion devices, physical optics, computer simulations

1. INTRODUCTION

Computer simulation codes play currently a decisive role in the development of modern light source facilities – storage ring based synchrotron radiation sources and linac based free-electron lasers. High-accuracy simulations by particle-tracking accelerator physics codes (see e.g. [1], [2]) greatly contributed to the progress made over the recent years in reduction of electron beam emittance in electron storage rings, down to ~100 pm level, and, as a consequence, very impressive increase of brightness of light sources based on these rings [3] - [5]. Simulation of multi-particle dynamics and impedance-related effects based on numerical solution of the associated electrodynamics problems in 2D and in 3D [6] facilitate detailed optimization of vacuum, RF, injection systems of these accelerators, and, as a result, enable stable operation of modern storage ring based sources at a high (~0.5 A in medium energy rings) average electron current, and the corresponding high average flux of the output Synchrotron Radiation (SR).

However, accelerator physics codes are not sufficient for the design and optimization of modern light source facilities. A very important place in the panoply of the software addressing these purposes is taken by the high-accuracy 3D magnetostatics codes dedicated for magnetic design of Insertion Devices (IDs) – undulators and wigglers – producing the radiation [7], and the electrodynamics codes that can accurately calculate all key characteristics of the SR generated by relativistic electrons in these magnetic fields [8] - [11]. A detailed knowledge of the SR characteristics is nevertheless still not sufficient for making use of this radiation in experiments. The emitted radiation has to be transported to experimental samples by optical systems of beamlines that have to be optimized and be of sufficient quality to not deteriorate important characteristics of the radiation beams, such as brightness and coherence, during this transport. The radiation transport, or propagation through individual optical elements and spaces in a beamline, has therefore to be simulated in detail, and this simulation has to be used as a basis for the optical system optimization prior to its practical realization.

The modern light source facilities – ultra-small electron beam emittance storage rings and, even more so, free-electron lasers – produce significant portions of coherent radiation, even at very small wavelengths belonging to hard X-ray range, and further increase of the radiation degree of coherence represents one of the main strategic goals for future development of these sources.

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X-ray optical simulations supporting advanced commissioning of the coherent hard X-ray beamline at NSLS-II

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ABSTRACT

We present the application of fully- and partially-coherent synchrotron radiation wavefront propagation simulation functions, implemented in the "Synchrotron Radiation Workshop" computer code, to create a 'virtual beamline' mimicking the Coherent Hard X-ray scattering beamline at NSLS-II. The beamline simulation includes all optical beamline components, such as the insertion device, mirror with metrology data, slits, double crystal monochromator and refractive focusing elements (compound refractive lenses and kinoform lenses). A feature of this beamline is the exploitation of X-ray beam coherence, boosted by the low-emittance NSLS-II storage-ring, for techniques such as X-ray Photon Correlation Spectroscopy or Coherent Diffraction Imaging. The key performance parameters are the degree of X-ray beam coherence and photon flux, and the trade-off between them needs to guide the beamline settings for specific experimental requirements. Simulations of key performance parameters are compared to measurements obtained during beamline commissioning, and include the spectral flux of the undulator source, the degree of transverse coherence as well as focal spot sizes.

Keywords: wavefront propagation simulation, X-ray optics, partial coherence, undulator source, transverse coherence

1. INTRODUCTION

Exploiting the coherence properties in the hard X-ray regime is an emerging theme at ultra-low-emittance synchrotron storage rings. The techniques making use of the X-ray transverse coherence include Coherent Diffraction Imaging (CDI) in both Bragg and forward scattering geometries and time resolved coherent scattering such as X-ray Photon Correlation Spectroscopy[1] (XPCS) or X-ray Speckle Visibility Spectroscopy[2] (XSVS). At a synchrotron source, the transvers coherence length of the X-ray beam in the hard X-ray regime is typically smaller than the phase space used in the experiments. Simulations of beamlines and experiments in these conditions therefore require partially coherent wavefront propagation methods. The simulations presented here use both the Python and browser based[3] (Sirepo, RadiaSoft LLC) implementations of Synchrotron Radiation Workshop (SRW)[4,5] to simulate beamline performance in the partial coherence regime. A 'virtual beamline' has been implemented, mimicking the characteristics of the Coherent Hard X-ray (CHX) beamline at the National Synchrotron Light Source II (NSLS-II). The main mission of the CHX beamline is the investigation of dynamics, or electron density fluctuations, in materials on length scales ranging from micrometer to Angstroms via XPCS or XSVS. Both XPCS and XSVS are the analogs of the corresponding techniques in the optical wavelength regime. X-ray wavelength give access to much smaller length scales, absorbing samples and buried interfaces. Typical samples investigated by XPCS and XSVS range from ferroelectric domains to complex fluids, polymer nanocomposites and bio-polymer gels. The requirements of XPCS and XSVS to time-resolve the length scale dependent dynamics by time series or 'snapshots' with acquisition times shorter than those of the dynamics rearrangements, make these techniques very photon hungry, in particular for fast dynamics at small length scales and/or weakly scattering samples. Both techniques are therefore used in the regime of partial transverse coherence, adjusting the phase space of the synchrotron source used in the experiments to the best compromise between the degree of transverse coherence and photon flux. Accordingly, the CHX beamline was designed to easily accomplish this trade-off and allow for optimizing conditions for each individual experiment. Partially coherent wavefront propagation simulations in SRW were used during the design phase to predict and optimize beamline performance. The effects of a non-ideal mirror height profiles and monochromator crystal imperfections were previously assessed by partially coherent wavefront propagation simulations and compared with data obtained during early beamline commissioning[6]. Other figures of merit that were evaluated via simulations during the design phase include the flux at the sample position, the focal spot size that determines the speckle size in coherent scattering pattern and the degree of transverse coherence for different beamline configurations.

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Alignment of KB mirrors with at-wavelength metrology tool simulated using SRW

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ABSTRACT

Synchrotron Radiation Workshop (SRW) is a powerful synchrotron radiation simulation tool and has been widely used at synchrotron facilities all over the world. During the last decade, many types of X-ray wavefront sensors have been developed and used. In this work, we present our recent effort on the development of at-wavelength metrology simulation based on SRW mainly focused on the Hartmann Wavefront Sensor (HWS). Various conditions have been studied to verify that the simulated HWS is performing as expected in terms of accuracy. This at-wavelength metrology simulation tool is then used to align KB mirrors by minimizing the wavefront aberrations. We will present our optimization process to perform an 'in situ' alignment using conditions as close as possible to the real experiments (KB mirrors with different levels of figure errors or different misalignment geometry).

Keywords: SRW simulation, at-wavelength metrology, X-ray wavefront sensor, X-ray mirror, 'in situ' alignment

1. INTRODUCTION

X-ray mirrors are extensively used both in synchrotron radiation and in table-top laboratory sources in order to collimate or to focus X-ray beams with high efficiency. The improvement in their fabrication technology allows now the manufacturing of quite long X-ray mirrors with rms slope error smaller than 50 nrad, sub-nm rms shape error and with rms roughness smaller than 0.1 nm. Using Kirkpatrick-Baez (KB) geometry, these mirrors can provide diffraction limited spot size smaller than 20 nm at 0.1 nm wavelength [1, 2].

However, reaching this level of spatial resolution obviously requires optimization of the alignment of the whole optical set up and high stability and the mechanical system. In parallel, virtual experiments through computer simulations have gained in popularity in recent years. The results of such simulations reproduce real experiments very well, thus it is becoming easier to make accurate and precise predictions about the outcomes of proposed experiments and to optimize beamline setups to achieve better performance.

The arrangement of two mirrors in a KB configuration [3] is widely used to achieve very small focus sizes reaching the diffraction limit for very short wavelength. In a KB system, the two elliptical cylindrical mirrors are orthogonal to each other and each mirror focuses the X-ray beam in a single plane. In order to reach a diffraction limited spot size, the rms shape errors of the mirrors must be lower than $\lambda/(28\cdot\theta)$ rms where λ is the radiation wavelength and θ is the incidence angle. This level of mirror quality has been demonstrated and the smallest reported beam size is around 13 nm [1].

We have studied mirror alignment of KB optics with the goal of realizing a close loop alignment system using an at wavelength wavefront sensor. In this paper we report the simulation of a Hartmann Wavefront Sensor (HWS) as an instrument to detect aberrations in an X-ray optical system and the way that this HWS can be used to perform close loop alignment. This study was done using the SRW simulation code [4-6].

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Novel magnesium borides and their superconductivity†

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With the motivation of searching for new superconductors in the Mg–B system, we performed *ab initio* evolutionary searches for all the stable compounds in this binary system in the pressure range of 0–200 GPa. We found previously unknown, yet thermodynamically stable, compositions MgB_3 and Mg_3B_{10}. Experimentally known MgB_2 is stable in the entire pressure range 0–200 GPa, while MgB_7 and MgB_{12} are stable at pressures below 90 GPa and 35 GPa, respectively. We predict a reentrant behavior for MgB_4, which becomes unstable against decomposition into MgB_2 and MgB_7 at 4 GPa and then becomes stable above 61 GPa. We find ubiquity of phases with boron sandwich structures analogous to the AlB_2-type structure. However, with the exception of MgB_2, all other magnesium borides have low electron–phonon coupling constants λ of 0.32–0.39 and are predicted to have T_c below 3 K.

Introduction

Tremendous efforts have been made to design conventional superconductors with higher and higher critical temperatures.[1–5] It is also the main focus of theoretical and experimental studies to determine how high the superconducting transition temperature T_c can be pushed in binary and ternary boron-compounds. For instance, theoretical studies predicted thermodynamically unstable CaB_2 to be superconducting at $\sim$50 K[1] and hole-doped LiBC to have T_c of 65 K.[2] Ternary Mo_2Re_3B with T_c = 8.5 K,[3] $CuB_{2-x}C_x$ (T_c ~ 50 K)[4] and the multiple-phase bulk sample of yttrium-palladium-boron-carbon (T_c = 23 K[5]) are important boron-based superconductors.

The unexpected discovery of superconductivity in MgB_2 with high T_c = 39 K[6] has triggered a flurry of publications. In previous studies, superconductivity of MgB_2 has been thoroughly investigated.[7–11] The isotope effect demonstrated the phonon-mediated nature of superconductivity in this compound.[12] Although doping is usually expressed as a hope to enhance the desired properties, carbon-doped MgB_2 ($Mg(B_{0.8}C_{0.2})_2$) has a lower T_c = 21.9 K.[13] Aluminum, with one more electron than magnesium, was reported to be an unfit candidate for partial substitution for magnesium ($Mg_{1-x}Al_xB_2$).[14] This shows that increasing electron concentration suppresses the superconductivity of magnesium diboride.

Elemental magnesium[15] and boron[16] have been shown to exhibit unexpected chemistry under high pressure, raising the motivation of studying their compounds. Moreover, materials composed of light atoms could make good conventional superconductors. The Mg–B system was subjected to some explorations of superconductivity.[17–19] Stability of boron-rich magnesium borides, *e.g.*, MgB_7, MgB_{12} and $Mg_{\sim5}B_{44}$, has been extensively studied by experiment at ambient pressure.[20] Borides of similar metals, *e.g.*, Ca–B[21] and Li–B,[22] and the stability of 41 metal borides[23] were studied and new compounds were shown to appear at high pressure. The high-pressure phase of MgB_2 (KHg_2-type structure) was reported to be a poor metal with no superconductivity, highlighting the main role of delocalized bonding of the boron honeycomb layers in the superconducting properties of MgB_2 with the AlB_2-type structure.[18]

To date, no comprehensive and systematic theoretical research has been reported on the stability and properties of magnesium borides at high pressure. Here, with the knowledge of the important role of magnesium,[13] the crucial existence of honeycomb boron layers[18] and the substantial effect of electron concentration,[14] we present results of extensive computational searches for stable magnesium borides Mg_xB_y and their superconductivity.

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ANALYSIS AND CORRECTION OF IN-VACUUM UNDULATOR MISALIGNMENT EFFECTS IN A STORAGE RING SYNCHROTRON RADIATION SOURCE*

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Abstract

In-vacuum undulators (IVU) are currently extensively used at light source facilities, in particular in medium-energy storage rings, for the production of high-brightness and high-flux hard X-rays. The relatively small (~5 mm or less) vertical magnetic gaps used in these planar undulators make them rather sensitive to the accuracy of the alignment of magnet arrays with respect to the electron orbit in the vertical plane. Based on commissioning results of hard X-ray beamlines at NSLS-II, misalignment of IVU with respect to the electron beam was found to be frequent among the reasons for spectral "underperformance". We present results of analyses of different IVU misalignment effects on the magnetic field "seen" by the electron beam and on the emitted undulator radiation spectra. An example of applying spectrum-based IVU alignment, which resulted in a ~2-fold increase in spectral flux at one of the NSLS-II beamlines, is presented.

INTRODUCTION

Achieving maximal-possible spectral performance is an obvious goal of the optimization, design, construction and commissioning of undulators at light source facilities. A considerable improvement of spectral performance of undulator sources was made thanks to the invention of permanent-magnet and hybrid IVU [1-3]. These Insertion Devices (ID) allowed for reducing the minimum magnetic gaps down to very small values (less than 5 mm). This enabled using small magnetic periods (around 20 mm and less) and yet creating high enough magnetic fields for reaching deflection parameter values K ~ 2 and so providing high-intensity Undulator Radiation (UR) spectra in the X-ray spectral range in medium- and high-energy storage rings. Due to the use of small magnetic gaps and relatively high spectral harmonic numbers (up to 15-25 in medium-energy rings), the spectra of these undulators are, however, very sensitive to the quality of their magnetic fields, which depends on the quality of permanent magnets, shimming, and on undulator alignment with respect to the electron beam.

After shimming and final magnetic measurements but before the start of use as a radiation source at a beamline, an IVU undergoes a number of operations that may potentially affect the quality of its magnetic field "seen" by the electron beam. This includes transport, installation, mechanical alignment, vacuum baking, etc. All these operations may result in imperfect alignment of IVU magnet girders with respect to the electron beam trajectory, as well as in mutual misalignment of the girders with respect to each other, that may take place after the final magnetic measurements and hence would not have been seen before installation. This misalignment may reach hundreds of microns in vertical position and tens (or hundreds) of micro-radians in vertical angle. Whereas for large-gap out-of-vacuum undulators such misalignment might not pose significant problems, it may considerably impact the spectral performance of small-gap IVUs in low-emittance storage rings.

During the initial commissioning with electron beam, an IVU typically undergoes some alignment procedures with respect to the beam. However, this alignment usually has a goal of minimizing negative effects of the IVU on electron beam dynamics (closed-orbit distortion, dynamic aperture, lifetime, etc.). This does not guarantee the highest-possible quality of the emitted UR spectra, since an imperfect undulator alignment may have considerably more severe effects on the resulting spectra than on the electron beam. Analysis of such effects and a search for the best strategies for their compensation are the main subjects of this paper.

SIMULATED IMPACTS OF UNDULATOR MISALIGNMENT

A schematics of a general misalignment case of a planar undulator (or wiggler) with respect to average electron trajectory passing through it is illustrated in Fig. 1. Two slightly non-parallel bold bars represent the undulator magnet arrays that have some vertical gap taper between them. This taper can be characterized by the gap variation between the undulator exit and entrance, $\Delta g = g_2 - g_1$, or by tapering angle $\Delta g/L_u$, where L_u is the undulator length. Besides the gap taper, the undulator has some vertical tilt angle θ between its median plane and the electron trajectory, and some vertical offset / "elevation" Δh of its magnetic center from the electron trajectory.

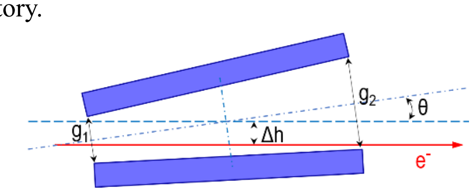

Figure 1: A general misalignment case of a planar undulator with respect to average electron trajectory and parameters used for characterizing this misalignment.

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A COMPREHENSIVE STUDY OF THE MICROWAVE INSTABILITY*

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Abstract

Several instability thresholds and special waveform beam patterns have been observed during measurements of the horizontal beam size change vs. single bunch current by the synchrotron light monitor (SLM) camera installed in a low dispersion area of the NSLS-II storage ring. The electron beam energy spread from the In-Vacuum Undulator (IVU) of the Soft Matter Interfaces (SMI) beam line confirmed the microwave beam pattern behaviour as a current dependent effect. The numerically obtained total longitudinal wakepotential by the GdfidL code allowed us to compare the measured results with particle tracking simulations using the SPACE code. The instability thresholds behaviour at different RF voltages are in some sort of overarching agreement.

SLM AND IVU SPECTRA MEASUREMENTS

The new generations of storage ring light sources do not offer any reduction of another important "part" of the full 6-dimensional electron beam emittance – the energy spread. Electron beam energy spread is an important limiting factor for the peak flux at spectral harmonics of undulators – the main insertion devices used as radiation sources in these storage rings. Besides reducing the spectral flux, especially at high undulator radiation harmonics that are extensively used for producing X-rays in medium-energy storage rings, the electron beam energy spread affects angular divergence of the emitted radiation, and can represent a significant obstacle for the increase of undulator radiation brightness in future ultra-low-emittance storage ring based sources. A detailed study of electron beam energy spread in different operation regimes represents a very important topic of electron beam dynamics studies in storage ring facilities.

Two diagnostic methods have been applied to measure the longitudinal microwave beam instability thresholds and its microwave pattern behaviour in the NSLS-II storage ring: 1) the horizontal beam-profile change versus single bunch current has been monitored by a SLM camera installed in a low dispersion area [1], and 2) the In-Vacuum Undulator (IVU) of the Soft Matter Interfaces (SMI) beam line [2] has been used as a diagnostic tool to determine the full width at half maximum (FWHM) change as a function of current based on the IVU spectrum of 7th harmonic.

Horizontal beam size and FHWM of IVU spectra as a function of single bunch current are shown in Fig. 1 for two different lattices: 1) bare lattice (BL), with all insertion devices (IDs) magnet gap open and 2) 3DW lattice, with all IDs magnet gap closed. Measurements by the SLM camera were done during different studies time and they are repeatable. The designed energy spread (in the limit of zero beam intensity) in NSLS-II can be varied by closing and opening the magnet gaps of three 7m damping wigglers (DWs) installed in Cell 08, 18, 28 [3].

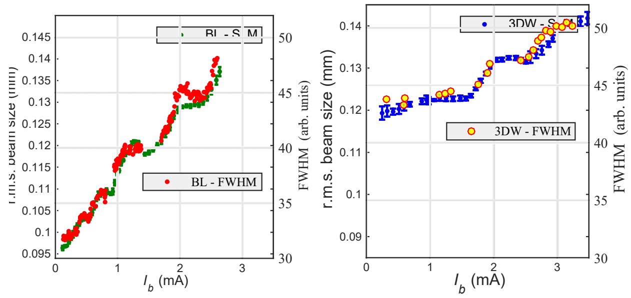
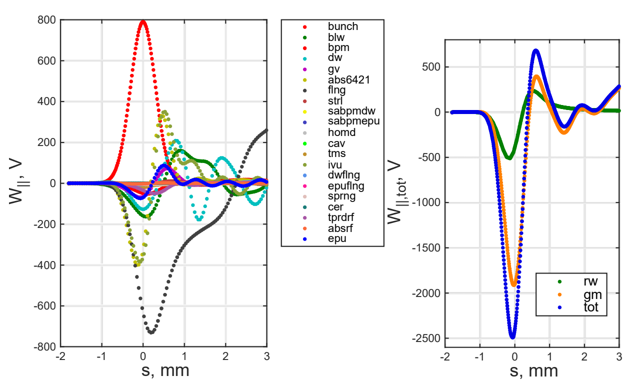


Figure 1: Horizontal beam size change measurements from SLM camera and FWHM measured form the IVU spectrum of 7th harmonic at $V_{RF} = 2.6MV$ for the two different lattices BL and 3DW.

IMPEDANCE BUDGET ($\bar{\sigma}_s = 0.3mm$)

To predict the longitudinal instability thresholds and bunch lengthening induced by the potential well distortion, the longitudinal wakepotential $W_{||}(s)$ is numerically calculated as a sum of the contributions due to vacuum chamber components distributed around the ring (Fig. 2a). An approximation to the wakepotential for a $\bar{\sigma}_s = 0.3mm$ charge distribution length, much shorter than the length of the unperturbed circulating bunch is used as a pseudo-Green's function for beam dynamic simulations (Fig. 2b).



a) b)

Figure 2: The longitudinal short-range wakepotential calculated for a $\bar{\sigma}_s = 0.3mm$ bunch length. a) $W_{||}(s)$ calculated for each individual vacuum component and multiplied by a total number. b) The total longitudinal wakepotential $W_{||,tot}(s)$ of the NSLS-II storage ring as a sum of geometric and resistive wall wakepotentials.

The 3D GdfidL numerical code has been used for the wakepotential simulations [4]. Not all vacuum compo-

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ALLOYING EFFECTS ON THERMODYNAMIC CHARACTERISTICS OF HYDROGEN IN BCC IRON

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Substitutional impurities have significant effect on hydrogen behaviour in iron. It opens a possibility to control hydrogen degradation of steels through directional alloying. The paper contains a review of theoretical and experimental studies of the problem of trapping of hydrogen atoms by alloy impurities and using this effect for preventing hydrogen embrittlement. Influence of 3*d*, 4*d* and *sp* metals on the energy of solution of hydrogen in BCC iron matrix is then investigated by means of WIEN-2k software package realizing the linear augmented plane wave (LAPW), a full-electronic method of the density functional theory. Detailed consideration of the change of equilibrium lattice parameter due to hydrogen dissolution in the alloyed BCC iron lattice is performed. The issue of alloy effect on preferred filling by hydrogen of tetrahedral and octahedral sites of interstitial sublattice is studied. Electronic and elastic contributions to the energy of solution are isolated. Energies of hydrogen trapping by impurity atoms are calculated, and significant contributions of both electronic and elastic effects to the trapping energy are demonstrated. It is shown that the change of the energy of solution of hydrogen due to impurities may be linked with the disturbance that they create in the electronic density of the matrix.

Keywords: alpha iron; hydrogen; substitutional impurities; trapping energy; first-principles modelling.

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