# DEVELOPMENT OF AN APPROACH TO MINIMIZE THE EFFECTS OF X-RAY GLITCHES


N. Klimova[1], O. Yefanov[2], A. Snigirev[1].

[1] IRC "Coherent X-ray optics for Megascience facilities", IKBFU, Kaliningrad, Russia.
[2] Center for Free-Electron Laser Science, Hamburg, Germany.


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Immanuel Kant Baltic Federal University

IRC "Coherent X-ray optics for Megascience facilities"

CFEL SCIENCE

## Abstract


Effective optics is crucial to realize all the possibilities and fully reveal the potential of 4th generation synchrotron sources. Compound refractive lenses (CRL) [1] are commonly used for focusing x-rays at synchrotrons due to easy alignment and good focusing efficiency. Diamond CRLs have low absorption, high heat conductivity and are well reproducible, that makes such lenses a perfect candidate for different type of experiments that require high focusing. Unfortunately optics, made of single crystal material, has one drawback that was recently reported [2] - intensity modulation at certain energies in the transmission spectrum. This issue is well known in X-ray spectroscopy and is called "diffraction loss" or "glitch effect" [3]. It is especially bad for spectroscopic experiments, where a certain energy range has to be scanned. **Glitches are always present in the transmission spectrum of single-crystal materials. It is necessary to develop such approaches that made it possible to conduct experimental studies with minimizing the effects of their influence.**


## Background

In papers [2, 4] X-rays were propagating through lenses, while the transmitted intensity was measured at different energies. The magnitude of the effect was then minimized down to ~ 10% by use of CRLs compiled from individual lenses with different crystallographic orientation. **At the same time, X-ray glitches did not affect any focal spot size or shape while only arousing the darkening of the focal spot at exact energies of X-ray glitches.**

## Experimental setups

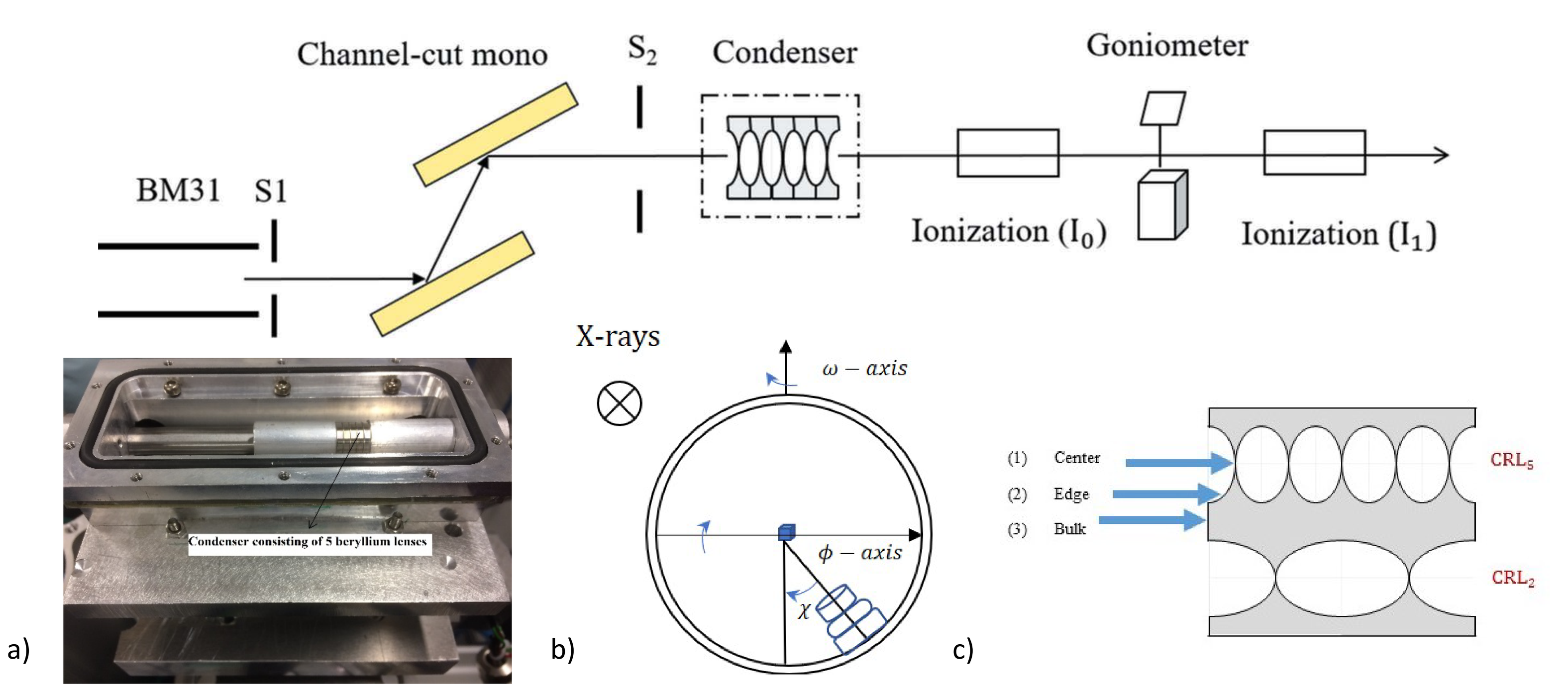



Fig. 1. "EXAFS" scan - Glitch spectroscopy of diamond lenses at BM31, SNBL ESRF: (a) is a picture of the condenser; (b) is the view of χ-angle from X-ray source in Eulerian geometry with ω=0°; (c) shows the impingement of the X-rays with the (1) center, (2) edge and (3) bulk material of diamond lenses, respectively (from top to bottom)

## Results

In [5-6], it was found that the spatial position of the incident X-ray beam (relative to the lens aperture) affects the intensity and position of the glitches. The value of the glitch intensity strongly depends on the thickness of the test sample, which is associated with the effect of attenuation (extinction) i.e. as the thickness of the material increases, the bigger fraction of incident radiation diffracts, so less is left in the transmitted beam. This causes a decrease in the intensity passing through the lens.

**Glitches become more pronounced with increasing thickness of the material through which the x-rays pass.**

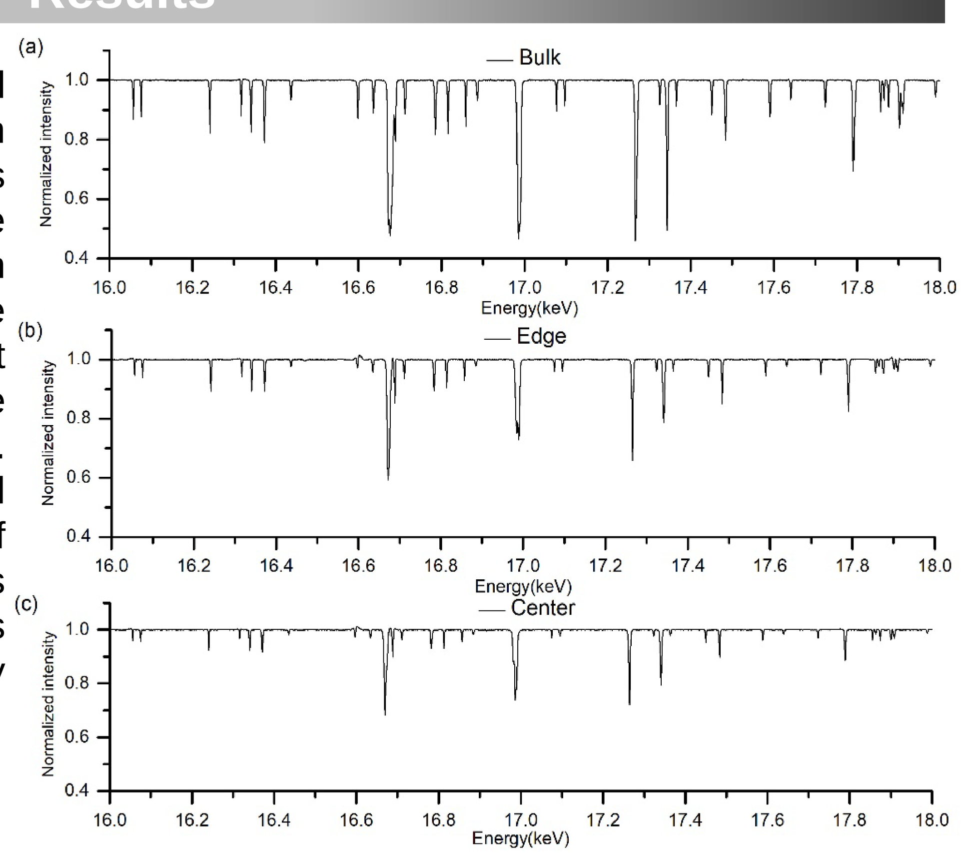
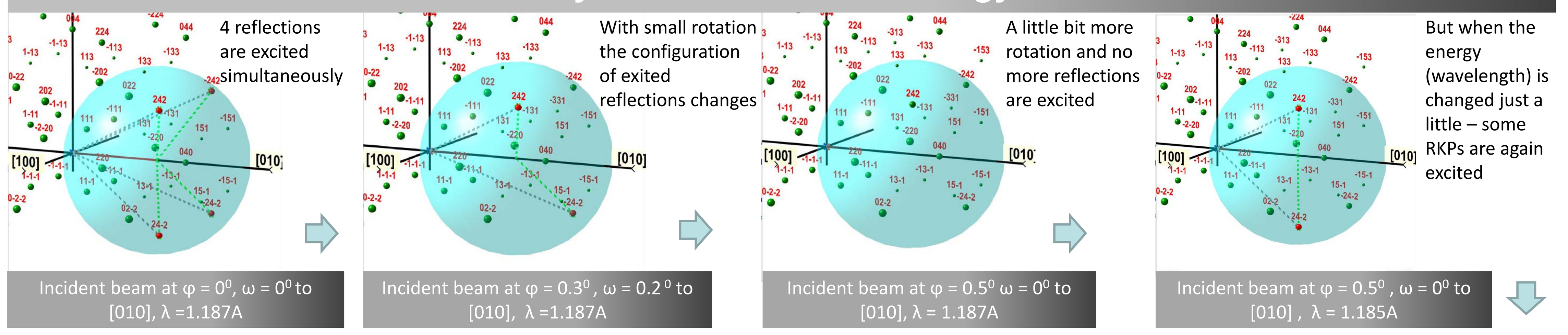



Fig. 2. The transmission spectra by confining X-ray to interact with (a) bulk, (b) edge and (c) center of $CRL_5$, respectively.

## Glitch sensitivity to incident beam energy and direction




The spectrum of glitches (that appear at a certain energy) is very sensitive to the orientation of the crystal relative to the incident beam, i.e. glitches occur at different frequencies, and if at 1⁰, for example, at an energy of 12 keV there is a glitch, then it already shifts by 0.2⁰, and this, in turn, may mean that a small rotation of the lens (along both axes) can eliminate glitches at the required energy.

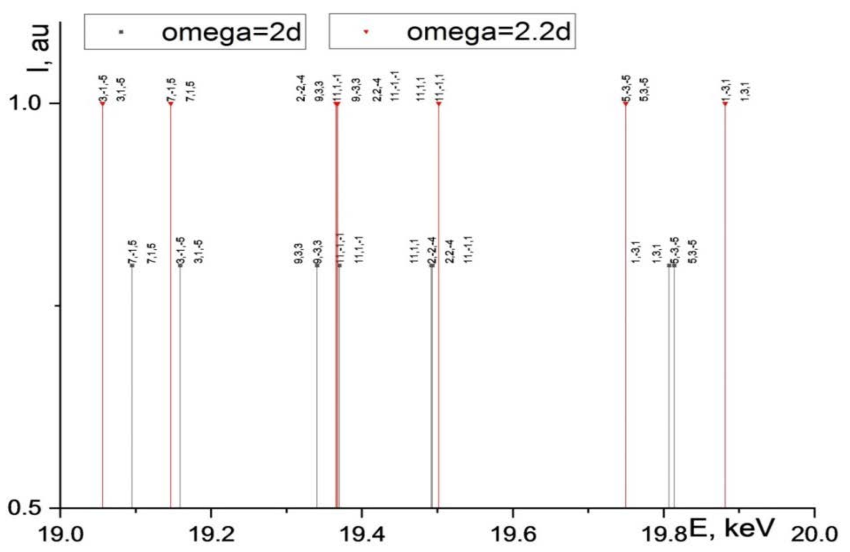



Fig. 4. Two glitch spectra with a difference of the angle of incidence of 0.2 degree.

**So it is easy to see in reciprocal space that excited RLPs strongly depend on the incident beam energy and direction**

## The procedure of predicting the glitches

The developed fitting procedure allows to predict the spectrum of glitches with high accuracy – see Fig. 5

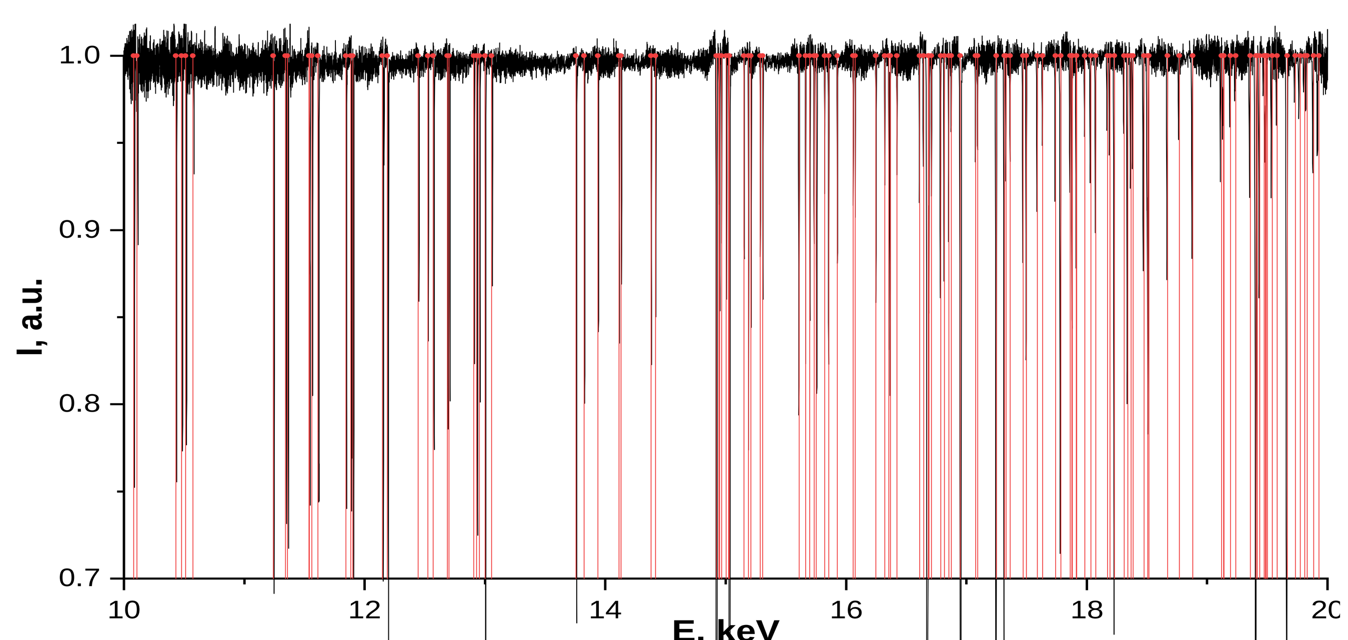



Fig. 5. Simulated spectrum of glitches (red) overlapped with the experimentally measured (black)

An important result of the proposed work is a theoretical model, which was confirmed by the experimental results and which allows predicting the position and strength (intensity) of glitches if the crystallographic orientation relative to the x-ray beam is known with sufficient accuracy.

At the incidence angles ω = 4⁰ and ϕ = 4⁰ the experimental spectrum of glitches is well reproduced. Much better than before [5,6] with only ω = 3.2⁰

## How to avoid glitches?

Determining the current orientation and cell parameter of the lens:

1) measure the energy of several glitches (at least 3) with high precision. Then find the orientation of the lens (it can be fitted by tilting possible $K_0$ directions and comparing the resulting spectrum to the measured one);

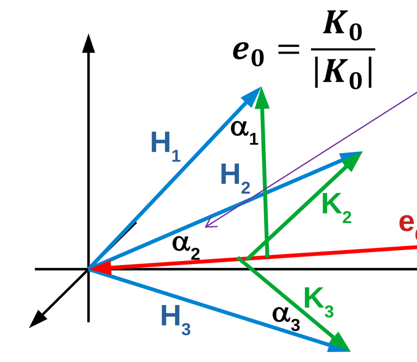
2) assign *hkl* indexes to the observed glitches ("indexing");

3) calculate analytically the exact direction of the incident beam and cell parameter.

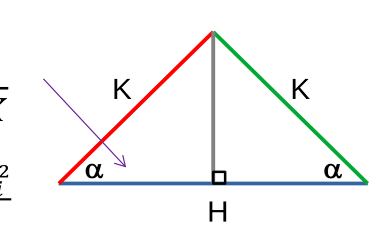
***This will allow to predict with high precision all glitches for current orientation.***

**Next multiple glitches spectra for different small tilts can be calculated, so for each energy a tilt with no glitches at that energy can be selected.**

When miller indices of several (>=3) glitches are determined, the true orientation of the lens with respect to the incident beam can be found.




$$\boldsymbol{e_0} = \frac{\boldsymbol{K_0}}{|\boldsymbol{K_0}|} \qquad \boldsymbol{e_0}\cdot\boldsymbol{H_2}=|\boldsymbol{H_2}|cos(\alpha_2) \qquad cos(\alpha) = \frac{H}{2K}$$




$$\boldsymbol{e_0}\cdot\boldsymbol{H_2} = \frac{H_2^2}{2K} \quad \text{With } K = \frac{E[keV]}{12.4}: \quad \boldsymbol{e_0}\cdot\boldsymbol{H_i} = \frac{6.2\,H_i^2}{E_i}$$

For cubic cell: $\boldsymbol{H} = a^*\,\overrightarrow{hkl}$ , so $H^2 = {a^*}^2(h^2+k^2+l^2) = a^*|\overrightarrow{hkl}|^2$

and $\boldsymbol{e_0}\cdot\overrightarrow{hkl}_{\boldsymbol{i}} = 6.2\,a^*(h^2+k^2+l^2)/E_i$

$$e_{0x}h_1 + e_{0y}k_1 + e_{0z}l_1 = 6.2\,a^*|\overrightarrow{hkl}|_1^2/E_1$$
$$e_{0x}h_1 + e_{0y}k_1 + e_{0z}l_1 = 6.2\,a^*|\overrightarrow{hkl}|_2^2/E_2$$
$$e_{0x}h_3 + e_{0y}k_3 + e_{0z}l_3 = 6.2\,a^*|\overrightarrow{hkl}|_3^2/E_3$$

$$\begin{pmatrix} h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 \\ h_3 & k_2 & l_3 \end{pmatrix}\begin{pmatrix} e_{0x} \\ e_{0y} \\ e_{0z} \end{pmatrix} = 6.2\,a^*\begin{pmatrix} |\overrightarrow{hkl}|_1^2/E_1 \\ |\overrightarrow{hkl}|_2^2/E_2 \\ |\overrightarrow{hkl}|_3^2/E_3 \end{pmatrix}$$

Vector $\boldsymbol{e_0}$ can be found. Then taking into account that $|\boldsymbol{e_0}|$=1, a* (and a=1/a*) can also be determined

## Explanation of glitshes formation

The x-ray beam of a certain energy, incident on a crystal, might satisfy the Bragg (or Laue) condition for some set of crystall planes. In this case diffraction occur and some part of the incident beam will be diffracted, therefore the intensity of the incident beam will be reduced. This process is easier to explain in reciprocal space – the diffraction occur when a reciprocal lattice point (RLP) is intersected by the Ewald sphere build for current experimental parameters (incident beam direction and energy). Fig. 4 explains the glitchs formation in both spaces

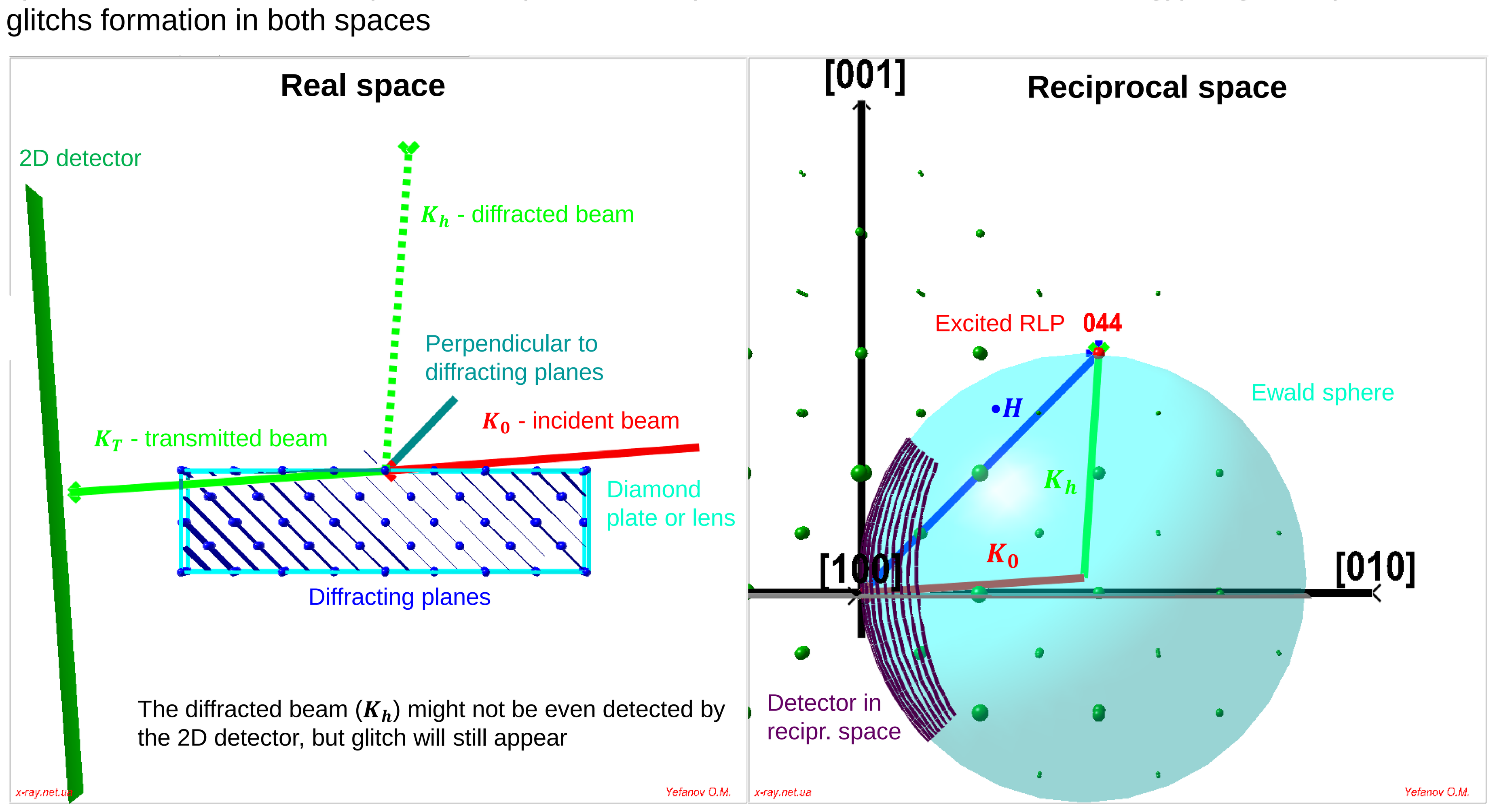



Fig. 3. The principle of glitch formation: when the Ewald sphere intersects some reflection a glitch appears in the transmitted beam*

## Conclusions

Results described in the papers:

- Glitches appear in the transmission spectrum that may cause a significant drop of intensity at some energies.
- The glitch positions (and corresponding strengths) may be predicted via the orientation matrix.
- The positions and strengths of glitches are very sensitive to orientation of the lens.
- The theoretical model allows one to predict glitch positions and strengths if the crystallographic orientation relative to the X-ray beam is known to an adequate precision.
- The beam divergence has a very limited influence on the transmission spectra
- The spatial position of the incident X-ray beam (relative to the lens aperture) effects the strength of glitches.
- This method is not restricted to single-crystal diamond, but can also be applied in other single-crystal optical devices.

Unpublished results:

1. Quantitative explanation of the experiment (good fit of experimental data with simulation)
2. Algorithm and program that can determine precise orientation of the lens solely from the spectrum of glitches
3. An analytical approach to refine the actual orientation of the lens and cell constant
4. The method of "getting rid" of glitches for each energy with the help of a small tilt of the lens. This tilt is easy to calculate based on points 2 and 3.
5. The "glitch free" usage of diamond lenses opens a way of using these focusing devices for any application that require continuous change of incident beam energy, including spectroscopy.

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*made by XVis http://x-ray.net.ua/xvis.html

Please contact nklimova@kantiana.ru or visit our page at https://www.cxoptics.ru for more information