Holography with γ-rays - Simulations vs. Experiment on α-^{57}Fe

P. Korecki
Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków, Poland

J.Korecki and W.Karaś
Department of Solid State Physics, Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy, 30-059 Kraków, Poland

The γ-ray holography was recently applied [P. Korecki *et al.* Phys. Rev. Lett. **79**, 3518 (1997)] to image the three-dimensional structure of α-^{57}Fe with an atomic resolution. A simple theory of the hologram formation based on Single Scattering Cluster formalism taking into account the polarization effects in the resonant nuclear scattering and absorption processes is presented. The high quality of the real-space reconstruction is demonstrated, however problems arising from the cancellation of real-twin images are revealed. The realistic simulations are in a good agreement with the experiment. A method for elimination of the real and twin-images cancellation taking advantage of the strong dependence of the scattering phase on the de-tuning from the resonance in the nuclear scattering is proposed.

76.80.+y, 07.85.-m, 42.40.-i

I. INTRODUCTION

In the previous paper,[1] we demonstrated experimentally the possibility of the γ radiation use for the holographic structure imaging on an atomic scale. The idea of so-called internal source holography (ISH) comes from Szöke[2] as the development of Gabor's[3] microscopic principle. A diffraction pattern formed by a radiation emitted from sources localized inside solids may be interpreted as a hologram. Such holograms can be formed by photoelectron or fluorescent X-rays emitted from internal sources excited by an external radiation (e.g. hard X-rays). For a radiation of a sufficiently short wavelength, the holographic real space reconstruction gives three-dimensional (3D) structure with an atomic resolution. In a simple wave picture, the wave directly reaching a far-field detector is taken as the holographic reference wave, whereas these ones being additionally scattered on the nearby atoms are treated as the object waves. The resulting interference pattern is recorded at once on a screen or collected point by point by moving the detector to cover a possibly high angular range. The holographic reconstruction is made numerically.[4]

The internal source holography was introduced using electrons: the photoelectrons, the Auger electrons and the low and medium-energy electrons elastically and non-elastically scattered.[5] Because the interaction of electrons with matter is strong, only surface layers can be imaged. Moreover, the electron-atom scattering as well as the electron emission may be strongly anisotropic and the multiple scattering and self-interference is involved, which causes that the reference and the object waves are ill defined. A considerable improvement of the real-space reconstruction quality is gained if the holograms are acquired for several different energies and if the multiple-energy reconstruction methods are applied.[6,7] One of the main advantages of multiple-energy measurements is the elimination of the twin images, which can hinder the proper determination of the structure.

Recently, also the X-ray holograms were presented.[8–10] Due to a high transparency of solids for X-rays, that kind of holography enables the imaging of bulk structures. On the other hand, the weak interaction implies that the holographic oscillations in the measured patterns are very weak and consequently the hologram acquisition time is long. The value of the Thomson scattering amplitude gives the typical holographic oscillations in the range of 0.1%-0.3% of the reference wave as compared to 30%-50% for the electron holograms.[11]

Up to now, two versions of the X-ray holography were performed. The direct one is called the X-ray Fluorescence Holography (XFH).[8] In the XFH the sample is excited by the external X-ray beam. An angular distribution of the following fluorescence from individual atoms (internal sources of the hologram) is measured using a far field detector. The method is limited to a predefined single energy and in addition, it requires a sufficiently low wavelength (high Z elements) to accomplish the atomic resolution.

Gog et al.[9] presented the Multiple Energy X-ray Holography (MEXH) being a time reversed version of the XFH. The MEXH principle uses the optical reciprocity theorem. Here, the positions of the source and the detector are interchanged. The atoms at crystal sites are microscopic holographic detectors, and the fluorescence measured in all directions is used only to probe the electromagnetic field inside a crystal at the position of the detector atom. The holographic pattern is formed due to the diffraction of the incident beam that causes a modulation of the total fluorescent yield measured as a function of the sample orientation relativ to the propagation direction of the incident radiation. Both kinds of holography, the direct and reversed one, will be called here the ISH.

The main advantage of the MEXH is the possibility of the multiple-energy measurements with the strong tunable synchrotron sources. By applying of multiple-energy reconstruction methods,[6,7] the twin-image problems can be overcome. As it was predicted theoretically,[11–13] for a certain combination of the atomic distances and the $\boldsymbol{k}$-vector values the overlapping of the real and twin images may lead to a suppression (enhancement) of the atomic images in the hologram reconstruction. These periodic effects are due to a different phase behavior of twin and real images. Another possibility to perform the multiple-energy experiments involving the Bremsstrahlung was proposed theoretically by Miller and Soerensen[14] in terms of QED.

The ISH can be also done with the γ-radiation. The idea comes from Tegze and Faigel[12] who proposed to use nuclear emitters inside a crystal. In that case, there is no need to use the external excitation source. There are two scattering maechanisms responsible for the hologram formation with the internal nuclear emitters. In the most direct way, a nuclear radiation could form holograms in similar scattering processes as in the X-ray holography. However, when the holography is performed with the γ-radiation, use of the strongest γ scattering process, namely the nuclear resonant scattering, becomes obvious. The processes of this type can be realized only by means of the Mössbauer effect. The resulting holographic pattern may be recorded in the far-field using a conventional γ-ray detector, with a moderate resolution. A parallel detection with a position sensitive detector could result in a huge reduction of the acquisition times, making them reasonable. The resonant detection using the moving Mössbauer absorber is also possible, which additionally brings the sensitivity to a magnetic order in the sample. The γ-ray holography can be also done in the inverse version and the first hologram obtained with the resonant scattering of the nuclear radiation in the reversed geometry was presented recently.[1]

In this paper we will discuss the essential features of the inverse version of the γ-ray holography (GRH) based on the simulated and experimentally obtained holograms and the real space reconstruction images of the α-^{57}Fe structure. The principles of the discussed version of the GRH are presented in Section II. Section III contains a simplified theory of the hologram formation taking into account the vector character of the used radiation and the resulting strong polarization effects. The holographic analysis will be reduced to the Single Scattering Cluster (SSC)[15] calculations. The small cluster calculations, reflecting the character of idealized holograms are given in Section IV. The calculations of the holograms and their reconstruction for the real experimental situation and a comparison with experimental results for a thin epitaxial ^{57}Fe film is presented in Section V, showing main physical and methodological limitations of the method. In Section VI we propose how to eliminate the cancellation of the real and twin images, being one of the weaknesses of the method. In Section VII we discuss the perspectives of the GRH for more complex systems.

II. PRINCIPLES OF THE INVERSE γ-RAY HOLOGRAPHY BASED ON THE RESONANCE DETECTION: 14.4 KEV ^{57}FE CASE TRANSITION.

In the discussed, inverse version of the GRH the photons from a conventional Mössbauer source (^{57}Co) are directed on to a sample containing the ^{57}Fe isotope, where they are resonantly absorbed by the nuclei. The excited nuclei can re-emit a γ-ray photon or deexcitate to the ground state trough the inelastic channel emitting a conversion electron. In the kinematical approximation the incident photon may be absorbed either directly (the holographic reference wave) or after being resonantly scattered on nearby nuclei (the object waves). The interference of both processes leads to the holographic oscillations in the total yield of the internal conversion electrons or other products of the decay emitted in the non-elastic channel. The electron yield is measured as a function of the incident angle of the external γ-ray beam. Obviously, a hologram will be formed only if the local surroundings of the absorbing nuclei are identical and equally oriented. It should be also pointed out that the so-called "atomic resolution" in the holographic reconstruction has to be thought as the average over the whole crystal.

Properties of the nuclear radiation and nuclear resonant scattering[16] make them very attractive for holography. For the 14.41 keV transition in ^{57}Fe the corresponding wavelength of 0.86Å is sufficiently short for atomic resolution. For this kind of radiation the nucleus can be treated as a point scatterer, so the form factor is constant. The angular anisotropy is caused only by the polarization effects and because the nuclear transitions in ^{57}Fe are M1, the scattering amplitude is a slow varying function of angles.

The amplitude and phase of the scattered radiation can be modified by the Doppler shift of the source energy, which enables also the tuning to only the recoil-free processes. Moreover, the excited state life time is long compared to the characteristic lattice vibration times of atoms in the sample and the Lamb-Mössbauer factor, describing the thermal effects for the case of slow scattering, is isotropic.[17] For magnetically ordered systems, the levels are split and the scattering and absorption is influenced by the internal magnetic fields at the nuclei. In consequence, there is a possibility to image only chosen nuclei, with a particular set of the hyperfine interaction parameters, and it is possible to resolve the 3D magnetic structure of the sample.

In the case of ^{57}Fe the conversion coefficient α, responsible for the ratio of the non-radiative to radiative decay probability, is 8.17. This value is almost ideal for the holographic application with the detection through the inelastic channel. The detection of conversion electrons is very efficient. The electrons following the conversion process are easy to detect over a full hemi-sphere above the sample using a simple proportional detector. On the other hand, the α determines the scattering strength given roughly by $\lambda\Gamma_\gamma/\Gamma = \lambda/(1+\alpha)$, where λ is the radiation wavelength and Γ_γ, Γ are the radiative and total excited level widths, respectively. The nuclear resonant scattering amplitude value is still very high as compared to the X-ray Thomson scattering amplitude given in the forward direction by Zr_0, where Z is the atomic number and r_0 is the classical electron radius. In a sharp resonance, the value[15] of the nuclear resonant amplitude can be as high as $\sim 440r_0$ for ^{57}Fe and may cause holographic oscillations of several percents in the measured pattern. The γ radiation scatters on electron shells as well, but those processes are much weaker than the nuclear scattering.

The holographic pattern can also reveal strong features caused by the long-range coherent effect. In the case of internal crystal emitters, they are observed as the Kossel lines or standing wave pattern.[18–20] The dynamical coherent long-range features may play an important role in the case of nearly perfect crystals, where the effect of an anomalous low nuclear absorption (similar to the Bormann effect for X-rays[21]) was predicted.[22–24] This effect leads to a suppression of the inelastic channel and it was experimentally confirmed by Smirnov and Chumakov.[25] In an experimental geometry analogous to the geometry of the inverse holographic experiment,[1] a well collimated incident beam, irradiating a nearly perfect single-crystal at the Bragg angles, gave a 50% fall-off of the conversion electron yield. The observed features had a very sharp angular character. In the holographic experiment, a much lower collimation is allowed and ,additionally, the Bragg features may be eliminated when a low-pass filter is applied to the hologram,[8,9,12] especially when the sample is non-perfect. However, for a more complex system, electronic scattering, as well as the dynamical effects should be taken into account. They may significantly distort structure images in the holographic reconstruction.

III. HOLOGRAM FORMATION AND THE REAL SPACE RECONSTRUCTION

Kagan and Afanas'ev[22,23] explained the effect of an inelastic channel suppression in the nuclear absorption when a perfect sample is irradiated at near the Bragg angle. The suppression takes place when the total amplitude of the excited state formation is zero due to the cancellation of electromagnetic fields at nuclear sites. In our version of holography, the conversion electron emission is also involved, but the holographic oscillations are the consequence of the short-range order. The nuclear excitation amplitude at a chosen crystal site is affected by the electromagnetic fields produced by excited nuclear resonators in the surrounding. In other words, the scattering of the γ-ray photon on nearby nuclei modifies the direct absorption. The modulation of the amplitude is observed when the external

γ-beam direction is scanned over the angles.

The formalism of the nuclear resonant scattering of the γ-radiation, needed for the description of the GRH is well known.[22–24,26–30] The scattering approach developed by Trammel and Hannon,[24] reduced to the kinematical approximation, is the most useful for our purpose. This single-scattering simplification is relevant for non-perfect crystals (small crystallites, mosaic structures etc.). For perfect crystals, the dynamical approach should be applied. The final formula for the hologram calculation will be given as a SSC equation, which allows to perform an easy test of the hologram and of the real-space reconstruction quality.

In the present calculation, we assume that a photon with a Lorenz frequency spectrum is emitted from a conventional ^{57}Co source and only one photon is irradiating the sample at a given moment. The source is moved with the constant velocity to tune to a particular nuclear transition. We neglect the modification of the photon spectrum in the source and in sample due to the absorption (thin source and absorber approximation). The photon can reach the absorbing nuclei on different paths, directly or after being single or multiple-scattered. Here, only the paths involving single scattering inside a cluster around the absorbing nuclei are considered (SSC model). We consider only these absorbing nuclei which deexcitate with the emission of a conversion electron and we assume that the conversion electron yield is proportional to the square of the total excitation amplitude. The conversion electrons coming from different nuclei are incoherent. The nuclear spin-flip scattering is also incoherent and therefore is not taken into account, as contributing only to the background. The emission from the ^{57}Co source is stochastic (time and space) and the individual photons are emitted with a random phase and polarization and the averaging over all photons should be performed.

We assume that the cluster represents a magnetically ordered and uniformly magnetized sample, containing ^{57}Fe. The magnetic splitting of the ground and excited states are large compared to the natural half-width and only one particular M1 transition may be considered.

Close to the resonance, the nuclear excitation amplitude due to a photon with the wave vector $\boldsymbol{k}$ and polarization $\boldsymbol{\eta}_p$ in a M1 transition is given by:[24,26]

$$S(\boldsymbol{k},\boldsymbol{\eta}_p) \propto \frac{C(j_g\,1\,j_e\,,m_g\,M\,m_e)}{E-E_{eg}+i\Gamma/2}\boldsymbol{Y}^{0}_{1M}(\hat{\boldsymbol{k}})^{*}\boldsymbol{\eta}_p \propto \frac{C(j_g\,1\,j_e\,,m_g\,M\,m_e)}{E-E_{eg}+i\Gamma/2}p\,D^{1}_{pM}(\hat{\boldsymbol{k}})^{*}, \tag{1}$$

where E is the energy of the incident photon, $E_{eg}=E_e-E_g$ is the transition energy between the ground and excited nuclear sub-levels, Γ and Γ_γ give the full and the radiative widths of the excited state, $\boldsymbol{Y}^{\lambda}_{LM}$ are the vectorial spherical harmonics ($L = 1$, $\lambda = 0$) and D^L_{pM} and $C(..)$ are the rotation matrices for $L = 1$ and the Clebsh-Gordan coefficient in notation of Rose.[31] The vectors $\boldsymbol{\eta}_{\pm} = \mp(\boldsymbol{e}_\theta \pm \boldsymbol{e}_\phi)/\sqrt{2}$ are the left and right circular polarization vectors, $p = \pm 1$ for $\boldsymbol{\eta}_{\pm}$, j_g, m_g, j_e, m_e are the quantum numbers of the ground and excited levels and $M = m_e - m_g$.

The total amplitude of the formation of the excited state may be written as a superposition of the excitation amplitudes by a plane wave from the source and by the spherical waves scattered on the nuclei inside the cluster. The scattered spherical wave is approximated by a plane wave with an amplitude and phase of the spherical one. This approximation, common in holographic applications, is particularly relevant for the nuclear scattering because of the small size of the nuclei.

For a given photon energy E and polarization $\boldsymbol{\eta}_p$ the total excitation amplitude is given by:

$$S_p^{tot}(E) \;=\; S_p^0(E) \;+\; \sum_i \sum_{p'=\pm 1} S^i_{p'}(E) \frac{f_i(\boldsymbol{k}_i\,\boldsymbol{\eta}_{p'}\,;\boldsymbol{k}_0\,\boldsymbol{\eta}_p)}{r_i}\, e^{i(k_0 r_i - \boldsymbol{k}_0\cdot\boldsymbol{r}_i)} \tag{2}$$

where $\boldsymbol{r}_i$ is the position of the i-th nuclei relative to the absorbing nuclei, $\boldsymbol{k}_0$ is the incident photon wave vector and $\boldsymbol{k}_i = k_0\boldsymbol{r}_i/r_i$, The exponential factor is responsible for the free propagation and it is assumed that the source is in the far field. The amplitudes S^0, S^i are the excitation amplitudes, the direct one and the one following the scattering on the i-th atom at the position $\boldsymbol{r}_i$, respectively:

$$S_p^0 = S(\boldsymbol{k}_0\,,\boldsymbol{\eta}_p)$$

$$S^i_{p'} = S(\boldsymbol{k}_i\,,\boldsymbol{\eta}_{p'}) \tag{3}$$

The scattering amplitude of the photon $(\boldsymbol{k}_0, \boldsymbol{\eta}_p)$ to a photon $(\boldsymbol{k}_i, \boldsymbol{\eta}_{p'})$ is the sum of the resonant nuclear scattering amplitude f_N and the Thomson scattering amplitude on electron shells f_E:[24]

$$f_i(\boldsymbol{k}_i\,\boldsymbol{\eta}_{p'}\,;\boldsymbol{k}_0\,\boldsymbol{\eta}_p) \;=\; f_N(\boldsymbol{k}_i\,\boldsymbol{\eta}_{p'}\,;\boldsymbol{k}_0\,\boldsymbol{\eta}_p) \;+\; f_E(\boldsymbol{k}_i\,\boldsymbol{\eta}_{p'}\,;\boldsymbol{k}_0\,\boldsymbol{\eta}_p) \tag{4}$$

The nuclear coherent resonant scattering amplitude is given by:

$$f_N(\boldsymbol{k}_i\,\boldsymbol{\eta}_{p'}\,;\boldsymbol{k}_0\,\boldsymbol{\eta}_p) \;=\; \frac{1}{2}\frac{3}{4k_0} f_{L-M} C^2(j_g\,1\,j_e\,,m_g\,M\,m_e)\Gamma_\gamma \frac{pp'\,D^1_{p'M}(\hat{\boldsymbol{k}}_i)D^1_{pM}(\hat{\boldsymbol{k}}_0)^*}{E_{eg} - E - i\Gamma/2}\,, \tag{5}$$

where f_{L-M} is the Lamb-Mössbauer factor and other symbols have been already described. The factor $1/2$ comes from the splitting of the ground state and stands for the inter-nuclear incoherence, whereas the Clebsh-Gordan coefficient is responsible for the intra-nuclear incoherence.

The Thomson scattering amplitude is given by:

$$f_E(\boldsymbol{k}_i\,\boldsymbol{\eta}_{p'}\,;\boldsymbol{k}_0\,\boldsymbol{\eta}_p) \;=\; -r_0 F^{el}(\theta_{scatt}) f_{D-W} \boldsymbol{\eta}^*_{p'} \cdot \boldsymbol{\eta}_p\,, \tag{6}$$

where r_0 is the classical electron radius, $F^{el}(\theta)$ is the atomic form factor, θ_{scatt} is the scattering angle between vectors $\boldsymbol{k}_0$ and $\boldsymbol{k}_i$, f_{D-W} is the Debye-Waller factor, and $\boldsymbol{\eta}^*_{p'} \cdot \boldsymbol{\eta}_p$ is the polarization factor.

To get the formula for the observed conversion electron yield $I(\boldsymbol{k}_0)$ an integration over the energy spectrum and summation over the polarization of the incident photon should be performed. Because the source is stochastic this can be made incoherently:

$$I(\boldsymbol{k}_0) \propto \int \sum_{p=\pm1} \left| S^0_p(E) + \sum_i \sum_{p'=\pm1} S^i_{p'}(E) \frac{f_i}{r_i}\, e^{i(k_0 r_i \,-\, \boldsymbol{k}_0 \cdot \boldsymbol{r}_i)} \right|^2 |A^0(E)|^2 \, dE \tag{7}$$

where:

$$A^0 \propto \frac{1}{E - (E_0 + E_s) + i\Gamma_s/2} \tag{8}$$

represents an energy spectrum of the incident photon, Γ_s is the total source line width (for the present calculation $\Gamma_s = \Gamma$) and E_0 is the source energy transition shifted due to the Doppler effect by $E_s = E_0 v/c$, where v is the velocity of the source.

Equation (7) may be rewritten using a "holographic" notation:

$$I(\boldsymbol{k}_0) \propto \int \sum_{p=\pm1} \left| r_p + o^N_p(E) + o^E_p \right|^2 \frac{C(\cdots)^2}{[(E-E_0-E_s)^2 + \Gamma_s^2/4][(E-E_{eg})^2 + \Gamma^2/4]} \tag{9}$$

where:

$$r_p = pD^1_{pM}(\boldsymbol{k}_0)^* \,, \tag{10}$$

$$o_N = \frac{3}{8k_0}\frac{pC(\cdots)\Gamma_\gamma f_{L-M}}{(E_{eg}-E-i\Gamma/2)}\sum_i\sum_{p'=\pm1}\frac{e^{i(k_0r_i-\boldsymbol{k}_0\cdot\boldsymbol{r}_i)}}{r_i}d^1_{p'M}(\theta_i)^2D^1_{pM}(\hat{\boldsymbol{k}}_0)^* \tag{11}$$

$$o_E = -\frac{e^2}{mc^2}\sum_i\sum_{p'=\pm1}F^{el}(\theta_{scatt})f_{D-W}\frac{e^{i(k_0r_i-\boldsymbol{k}_0\cdot\boldsymbol{r}_i)}}{r_i}p^{'}D^1_{p'M}(\hat{\boldsymbol{k}}_i)^*\boldsymbol{\eta}^*_{p'}\cdot\boldsymbol{\eta}_p \tag{12}$$

may be treated as the reference and the object waves (nuclear and electronic) for a given photon energy and polarization. Here, $d^1_{p'M}(\theta_i)$ is a real part of the rotation matrix $D^1_{p'M}$ and θ_i is the angle between the $\boldsymbol{r}_i$ vector, and the quantization axis. For compound samples, the summation in the o_N is over all nuclei equivalent to the absorbing nucleus and in the o_E over the all atoms in a cluster. It is seen from Eqns (10-12) that the measured pattern is an incoherent weighted sum of the individual holograms for a given spectral component of the incident photon.

The total conversion electron yield given by (9) may be written as the sum of a slowly varying "background" $I_0(\boldsymbol{k}_0)$, an oscillating term containing holographic information $H(\boldsymbol{k}_0)$ and higher order terms:

$$I_0(\boldsymbol{k}_0) \;=\; C(\cdots)^2F_M(\theta_0)\left(\int\frac{dE}{[(E-E_0-E_s)^2+\Gamma_s^2/4][(E-E_{eg})^2+\Gamma^2/4]}\right) \tag{13}$$

$$H(\boldsymbol{k}_0) \;=\; H_N(\boldsymbol{k}_0)+H_E(\boldsymbol{k}_0) \tag{14}$$

The nuclear holographic information is contained in:

$$\begin{aligned}H_N(\boldsymbol{k}_0) \propto &\frac{3\pi}{8k_0}C(\cdots)^4\Gamma_\gamma f_{L-M}F_M(\theta_0)\sum_i\frac{e^{i(k_0r_i-\boldsymbol{k}_0\cdot\boldsymbol{r}_i)}}{r_i}F_M(\theta_i)\times\\ &\int\frac{dE}{[(E-E_0-E_s)^2+\Gamma_s^2/4][(E-E_{eg})^2+\Gamma^2/4][E_{eg}-E-i\Gamma/2]} \;+\; c.c\end{aligned} \tag{15}$$

whereas the $H_E(\boldsymbol{k}_0)$, responsible for the scattering on the electronic shell, is much weaker. In Eqns [13,15], θ_0 is the angle between the incident photon and the quantization axis.

The angular polarization factors $F_M(\theta)$are:

$$F_M(\theta) \;=\; \sum_{p=\pm1}d^1_{pM}(\theta)^2 \;=\; \begin{cases}\sin^2\theta, & M=0\\ \frac{1}{2}(\cos^2\theta+1), & M=\pm1\end{cases} \tag{16}$$

For clarity, the electronic term as well as the higher order terms are not written down explicitly, but are included in the calculation.

The most important nuclear holographic term may be written as:

$$H_N(\boldsymbol{k}_0) \propto \sum_i f_T(\boldsymbol{k}_0, \boldsymbol{r}_i, E_s) \frac{e^{i(k_0 r_i - \boldsymbol{k}_0 \cdot \boldsymbol{r}_i)}}{r_i} + c.c \tag{17}$$

where the quantity:

$$f_T(\boldsymbol{k}_0, \boldsymbol{r}_i, E_s) \;=\; F_M(\theta_0) F_M(\theta_i) f(E_s) \tag{18}$$

is introduced as the effective amplitude of the scattering and the absorption. It contains the summation over all polarization and spectral components of the incident and scattered photons.

The energy dependent factor in the effective scattering and absorption amplitude is a function of the energy shift E_s:

$$\begin{aligned} f(E_s) = {} & \frac{3\pi}{8k_0} C(\cdots)^4 \Gamma_\gamma f_{L-M} \times \\ & \int \frac{dE}{[(E-E_0-E_s)^2 + \Gamma_s^2/4][(E-E_{eg})^2 + \Gamma^2/4][E_{eg} - E - i\Gamma/2]} \; + \; c.c \end{aligned} \tag{19}$$

To observe the holographic oscillations the propagation direction of the incident photon is to be varied with respect to the crystallographic directions.

Equation (17) is similar to the equation derived and used by Barton[4] for the formulation of the hologram reconstruction procedure. In our case the $H(\boldsymbol{k}_0)$ describes the non normalized holographic oscillations of the total electron yield following the conversion process, superimposed on a slowly varying background described by Eq. (13).

The 3D structure can be obtained from the normalized hologram $\chi(\boldsymbol{k}_0)$ by a 2D-phased-Fourier transform:[4]

$$U(\boldsymbol{r}) \;=\; \iint_S \chi(\hat{\boldsymbol{k}}_0) e^{-i\boldsymbol{k}_0 \cdot \boldsymbol{r}} \, d\sigma_{\hat{\boldsymbol{k}}_0} \tag{20}$$

where:

$$\chi(\boldsymbol{k}_0) = \frac{I(\boldsymbol{k}_0) - I_0(\boldsymbol{k}_0)}{I_0(\boldsymbol{k}_0)} = \frac{H(\boldsymbol{k}_0)}{I_0(\boldsymbol{k}_0)} \tag{21}$$

Usually, the hologram is additionally multiplied by a window function in order to avoid spurious oscillations arising from a finite range of integration in the k-space. The real structure is then represented[7] by $|U(\boldsymbol{r})|$, $|U(\boldsymbol{r})|^2$ or by $|rU(\boldsymbol{r})|^2$, where the last expression takes into account the radial fall-off of the reference or scattered wave.

To eliminate the anisotropic character of the scattering, modified reconstruction algorithms were proposed and originally applied for the electron holography. One of them, the Scattered Wave Included Fourier Transform (SWIFT)[32] method may be easily applied for the γ-ray holography and the modified transform is given by:

$$U(\boldsymbol{r}) = \iint_S \frac{\chi(\hat{\boldsymbol{k}}_0)}{f(\boldsymbol{k}_0, \boldsymbol{r})^*} e^{-i\boldsymbol{k}_0 \cdot \boldsymbol{r}} \, d\sigma_{\hat{\boldsymbol{k}}_0} \tag{22}$$

where the $f(\boldsymbol{k}_0, \boldsymbol{r})$ is the scattering amplitude.

IV. BASIC PROPERTIES OF THE γ-RAY HOLOGRAM. CALCULATIONS FOR A SMALL CLUSTER

The γ-ray scattering differs considerably from the scattering of electrons and the scattering of X-rays above the absorption edge. The polarization effects, a strong energy dependence of the scattering amplitude close to the resonance, and its different angular character are the most pronounced dissimilarities. In this section, we are analyzing the character of the γ-ray hologram and the quality of the real space reconstruction based on the results obtained in the previous section. To analyze the basic holographic features the calculations are performed for a relatively small α-^{57}Fe cluster, constructed of only seven coordination spheres (89 nuclei, 6.23Å radius) around the absorbing nucleus. For the simplified case, it is easier to examine the properties of the hologram formed due to a local environment, independently of experimental conditions and of the effects being a consequence of the long-range periodicity in the crystal. The holograms are calculated for the full hemisphere in the $\boldsymbol{k}$-space, and it is assumed that the source is rotated to cover the full angular range. The center of the hologram corresponds to the direction normal to the surface ($k_x = 0,\ k_y = 0,\ k_z = k$). For the edges of the hologram the vector $\boldsymbol{k}$ lies in the surface plane and $\boldsymbol{k} = \boldsymbol{k}_{||}$.

Our calculations should be related directly to the real experimental situation.[1] The experimental conditions were optimized to get the best possible hologram (in the sense of the signal-to-noise ratio). It implies the choice of one particular nuclear transition out of six, which are possible in the case of the magnetically split levels in ^{57}Fe (Fig. 1(a)).

The choice of the transition should regard not only the intensity of the holographic oscillations but also the fact that certain nuclei, depending on the position relative to the quantization axis, may be not illuminated and consequently, not imaged. The geometry used for the calculation, depicted in Fig. 1(b), corresponds to the α-Fe sample with the normal direction [001], which is uniformly magnetized in-plane in the [010] direction. All patterns are calculated in the sharp resonance.

Fig. 1(c) shows the spatial dependence of the conversion electron yield, due to the direct absorption of γ-rays (without scattering effects). The patterns are calculated according to Eq. (13) for the transitions $\pm 1/2 \rightarrow \pm 3/2$ and $\pm 1/2 \rightarrow \pm 1/2$ ($M = 0$), respectively. The pattern for the transition $\pm 1/2 \rightarrow \pm 1/2$ has the same character as for the transition $\pm 1/2 \rightarrow \pm 3/2$ but is weaker because of the dependence on the Clebsh-Gordan coefficient. There is no dependence of the direct absorption on the azimuthal angle in the both presented patterns.

In the inverse holographic geometry, the direct nuclear absorption plays the role of the reference wave. The angular anisotropy of the direct absorption comes from the polarization term determining how strong the absorbing and scattering nuclei are illuminated by the reference wave coming directly from the external source. Obviously, this factor does not influence the normalized hologram intensity $\chi(\boldsymbol{k}_0)$ but for the $M = 0$ transitions may even cancel the total measured signal. More important for the determination of the amplitude of the holographic oscillation is to realize (from Fig. 1(c)), how the scattering nucleus at the specific lattice site illuminates the absorbing nucleus . This is described by the factor $F_M(\theta_i)$.

The patterns shown in Fig. 1(c) represent a dependence of the $F_M(\theta)$ on the angle $\theta = \arccos(k_y/k)$ between the photon wave vector (incident or scattered) and the quantization axis. In the pattern for the $M = 0$ transition (varying as the $\sin^2\theta$) there are directions with no emission or absorption present. In consequence, some nuclei would not be seen in the real space images obtained from the hologram taken for $M = 0$ transition. For the transition $M = \pm 1$ the dependence is described by $\cos^2\theta + 1$.

Fig. 2 shows the calculated holograms of seven coordination spheres of the α-^{57}Fe structure. The pure nuclear holograms for the transitions $M = \pm 1$ and $M = 0$ are presented in Figs 2(a) and 2(b), respectively. The hologram due to the Thomson scattering and subsequent nuclear absorption in the $M = +1$ transition is shown in Fig. 2(c). For comparison, an idealized hologram, calculated for the isotropic scattering and absorption and with the square of object wave terms neglected, is shown in Fig. 2(d). Such a "Gabor-like"[3] hologram is calculated for a constant value of the scattering amplitude phase $\phi = -\pi/2$. This value corresponds to the sharp nuclear resonant scattering.

The intensity of the holograms in Figs 2(a-c) is normalized (by the multiplication factors given in Fig. 2) to get the same contrast as for the square reference wave of Fig. 1(c). Inspecting the patterns in Fig. 1(c), it is seen that the direct absorption in the normal direction (which corresponds to the center of the patterns, most important from the experimental point of view), is stronger for the $M = 0$ than $M = 1$ transition. On the other hand one can see in Fig. 2 that the holographic signal is stronger for the $M = \pm 1$ transition. This can be understood when the angular dependence of the $F_M(\theta_i)$ is analyzed . For the α-Fe structure in our geometry, the nearest neighbors are in the off-normal directions relative to the absorbing nucleus (illuminated better in the $|M| = 1$ transitions). A signal caused by the scattering on nuclei lying in the normal direction (next nearest neighbors - better illuminated in the $M = 0$ transitions) is weaker due to the radial fall-off of the object waves. Thus, for this particular structure the holographic oscillations utilizing the $\pm 1/2 \to \pm 3/2$ transition are more intense and, additionally, are superimposed on a lower background, which makes the acquisition most efficient. The amplitude of the holographic oscillation may reach in this case 3% of the total measured conversion electron yield. Moreover, for this transition the nuclei in the neighborhood will be imaged almost isotropically, whereas in the case of the $M = 0$ transition the nuclei lying in the directions parallel to the quantization axis will not be seen in the real space images.

A direct comparison of the pure nuclear holograms with the idealized one from Fig. 2(d) proves their nearly optical properties. As there is no the form factor and due to the fact that the scattering phase shift is angle independent, the nuclear holograms are almost identical with the Gabor holograms. They should provide high-fidelity real-space images, while the images obtained from the single-energy electron holograms are of rather poor quality. The nuclear holographic oscillation is stronger than that of X-ray holograms which makes the acquisition times reasonable. Their quality is also certainly better than in the single-energy XFH.

The Thomson hologram shown in Fig. 2(c) is much weaker than the pure nuclear hologram in the sharp resonance. It is even much weaker than it could be expected from the direct comparison of the maximum values of the amplitudes derived from Eqs (5) and (6). Additionally, the effective scattering and absorption amplitude includes an integration over the photon Lorenz energy spectrum and this should again enhance the Thomson electronic scattering, which is energy independent. To explain the relative suppression of the electronic processes, the anisotropy of the atomic form factor has to be considered. It has a maximum in the forward direction. In other directions, the amplitude may be an order of magnitude weaker. In the holographic geometry, the absorbing nucleus is illuminated from all directions. For nuclear holograms, the scattering on several nuclei can contribute constructively or destructively due to the comparable strength of the scattering in all directions. For electronic scattering, in the most favorable case only one atom is in the preferential forward scattering direction.

It is interesting to note that the Thomson hologram (shown for $M = +1$) has a lower symmetry than the nuclear one. Asymmetries of a similar character were experimentally observed for the Bragg γ-ray scattering on a ^{57}Fe foil.[33] The asymmetries observed in our Thomson hologram result from complicated polarization effects present in E1 atomic scattering and subsequent M1 nuclear absorption process, and they are a direct consequence of the interference between the object and reference waves. Is should be pointed out that this hologram is quite different from the XFH one. The differences arise from the resonant detection by a polarized nuclear detector. However, the sum of the Thomson holograms obtained for $M = +1$ and $M = -1$ as well as the single $M = 0$ hologram have the same symmetry as the pure nuclear one. It corresponds to the symmetry of the crystal reduced by the magnetic field in the $\hat{\boldsymbol{y}}$ direction.

The real-space images of the cluster structure, obtained by applying the holographic transform (19) to the $M = \pm 1$ hologram from Fig. 2(a), are presented in Fig. 3. The figure shows the 2D slices of the 3D real-space structure. The imaged area is always 14x14Å^2 and the absorbing nucleus (the reference nucleus) occupies the 000 site. The nodes of the square grid indicate the lattice sites in the bcc structure. The plots are presented in linear inverted grayscale and no threshold for suppression of smaller intensities is used. Figs 3(a) and 3(b) show the (001) cuts parallel to the surface: at z=0 Å (containing the reference nucleus) and at z=1.43 Å (the distance corresponding to the inter-planar spacing in the α-Fe structure above the reference nucleus). The (100) vertical cut of the real-space in the distance 1.43Å from the emitter is shown in Fig. 3(c). The sample is magnetized in the [010] direction. There are distinct maxima at the crystal lattice sites but different nuclei are imaged with different intensities. The intensity depends on the nucleus positions relative to the quantization axis. This is connected with polarization effects in the scattering and absorption. As expected, the nuclei at positions 100 and 100 are imaged with lower intensities as their counterparts in the [010] direction. The correction for the anisotropy of the object waves can be done in the SWIFT method, which is very simple in this case. Because the factor $F_M(\theta_i)$ does not depend on integration variables in Eq. (22) the reconstructed image should be just divided by it. Fig. 4 shows a (001) real-space cut (as in Fig. 3(a)) after anisotropy correction. All nuclei equidistant from the absorbing nuclei are imaged now with the same intensity.

The real-space images in Figs 3 and 4 show also more frustrating features. The intensities of the imaged nuclei vary independently on the position relative to the quantization axis in a way, which can not be explained directly by a simple radial fall-off of the scattered waves. In the (001)plane of the reference nucleus, all nuclei inside the cluster are visible but the images of the more distant 110 (and symmetry equivalent) nuclei are stronger than those of 010 (even after SWIFT correction). In the planes above and below, effects that are even more spurious are observed. In Fig. 3(b), the nearest neighbor at position $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$ and the nucleus at position $\frac{3}{2}\,\frac{1}{2}\,\frac{1}{2}$ as well as the nuclei in the symmetry related positions are well imaged. However, the nuclei at the crystal site $\frac{3}{2}\,0\,\frac{1}{2}$ and the symmetry related ones are not visible. In addition, four strong features are artificially imaged near the unoccupied $11\frac{1}{2}$-type sites. They come from the strong images of the nuclei in 110-type positions, which show through the plane below. In the vertical (100) cut, the situation concerning visibility of different nuclei is similar but, due to the different vertical and in-plane spatial resolutions, the shape of imaged nuclei is elongated along the normal axis.

The effects described above are mostly due to the overlapping of the twin and real-images and they were discussed extensively in Refs 11,13. Because of a different phase behavior of the real and twin images, the intensity of a given atom/nucleus in the real-space image may oscillate as a function of its position relative to the reference atom/nucleus and the wavelength used for the hologram acquisition. For some values of r_i/λ, the reconstructed images can be enhanced, suppressed or even vanish completely. The oscillations of the image intensity for a nucleus at the position $+\boldsymbol{a}$ having a counterpart nucleus in $-\boldsymbol{a}$ are shown in Fig. 5.

The holographic pattern is very sensitive to the combination of the structural parameters and the radiation wavelength used. For the real situation the interplay of the real and twin images can hinder the proper structure determination as it was discussed above. Another combination could be much more favourable as it is shown on the example of the hologram calculated for a different hypothetical lattice constant a=3.02Å . The hologram (Fig. 6(a)) differs very much from that obtained for $a_{\alpha-Fe}$=2.87 Å (compare Fig. 2(a)). The (001) cut of the real-space is presented in Fig. 6(b). The reconstructed image is noticeably different as compared to the case for the true lattice constant (compare Fig. 3(b)). All nuclei in the plane above the reference nucleus are well imaged. This example shows that the problem of twin-images can be very troublesome in the γ-ray holography and the structure determination process can be ambiguous in the single-energy holography.

V. REAL SAMPLE - EXPERIMENT AND SIMULATIONS.

In this section, we will present a comparison between simulations and experimentally obtained data. Details of the experimental procedure were described previously.[1] The total yield of the electrons following the conversion processes was measured as a function of the sample orientation relative to the γ-rays propagation direction. The sample was a

2000Å ^{57}Fe film grown by the Molecular Beam Epitaxy on a polished 10x10x1mm^3 MgO(001) single crystal substrate. The film consisted of small equally oriented ^{57}Fe(001) crystallites. The average crystallite diameter was smaller than 100Å . The kinematical approximation in the calculation is for this sample appropriate and the dynamical effects should be considerably suppressed. The sample was magnetized along the in-plane [010] direction. The conventional 100 mCi ^{57}Co(Rh) Mössbauer source of 8mm diameter was placed 15cm from the sample. The hologram was acquired in the sharp resonance for the source Doppler tuned to the $M = \pm 1$ nuclear transitions. The data were normalized to an off-resonant signal. The angular pattern was recorded on a $d\theta_1 \times d\theta_2 = 1.80° \times 1.80°$ mesh in the range from $-43.2°$ to $43.2°$ for two angles of rotation around the [100] and [010] directions.

For comparison with the simulation, the normalized experimental pattern was transformed to the $\boldsymbol{k}$-vector mesh and then it was two-fold symmetrized. A slowly varying background intensity coming mainly from the reference wave was subtracted from the total signal $I(\boldsymbol{k}_0)$. In the background elimination process, the low-frequency gaussian convolution $I(\boldsymbol{k}_0) \otimes G(\boldsymbol{k}_0)$ was subtracted from the measured pattern giving the normalized hologram:[34]

$$\chi(\boldsymbol{k}_0) \;=\; I(\boldsymbol{k}_0) \;-\; I(\boldsymbol{k}_0) \otimes G(\boldsymbol{k}_0) \tag{23}$$

presented in Fig. 7(a).

The simulation of a real hologram was performed for a cluster of 300 coordination spheres ($\sim 10^4$ nuclei,$\sim$ 30Å radius) of the α-^{57}Fe structure on a coarse angular grid analogous to that one used in the experiment. In the simulation, the integration over the source and sample areas as well as the real source-to-sample distance were included. Due to this procedure the hologram becomes more blurred. The background (reference wave) removal was the same as in the case of the experimental data to take into account possible distortions of the real-space introduced by this procedure. The calculated hologram is presented in Fig. 7(a). The intensity distributions in the experimental and calculated holograms are very similar, especially when one keeps in mind a high sensitivity to the lattice parameter.

Differences in the relative intensities between the simulated and experimental holograms are probably due to the imperfect procedure of the background removal. When single profiles of the holograms are compared, the agreement between the experiment and the calculations is especially well emphasized, as can be seen from Fig. 7(b). The real-space images of the structure obtained by applying the holographic transform to the calculated and experimental holograms are shown in Figs 8(a-c) and 8(d-f), respectively. In both cases, the nearest neighbors in the α-Fe structure are well imaged. In cuts obtained from the experimental hologram, the images of the nearest neighbors are shifted by about 0.2Å from the true positions. It is caused by experimental errors in the sample orientation. The limited angular range used for the hologram recording results in a moderate resolution. The theoretical resolution is calculated according to Ref. 35 and it is shown as the vertical and horizontal bars on the plots. The poor vertical resolution makes the images of the $\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}$-type nuclei elongated along [001] axis in Figs 8(c) and 8(f). The overlapping of the real and twin images enhances this effect and in the (001) plane of the reference nucleus, the four maxima corresponding to "wings" of those nuclei are dominant. The images of all other nuclei beyond the first coordination shell are strongly suppressed. This is a consequence of a poor angular resolution, resulting from the relatively short source-sample distance and the finite size of the source and the sample, but also due to the coarse angular grid. It is however interesting to note, that the nuclei at $\frac{3}{2}\,\frac{1}{2}\,\frac{1}{2}$ and the symmetry equivalent sites are not imaged at all. This effect can be also observed in Fig. 3, for the idealized experimental situation, and it is clearly due to the cancellation of the real and twin images. Some differences of the relative intensity ratios in the experimental and theoretical real-space cuts may be also caused by the experimental error in tuning to the resonance energy. The phase of the scattering amplitude is a rapid function of the small shifts from the resonance energy, and the scattering phase determines the overlapping of real and twin images.

The resolution and the size of the imaged area can be improved by recording the hologram in a wider angular range, with a better angular resolution. The polarization effects are easy to be eliminated with the SWIFT method. So, the main limitation in the single-energy γ-ray holography remains the effect of the cancellation of the real and twin images.

VI. ELIMINATION OF REAL AND TWIN IMAGES CANCELLATION IN γ-RAY HOLOGRAPHY

In the case of the γ-ray holography utilizing the Mössbauer effect, it is possible to vary the energy of the incident beam only in a close vicinity of the resonance. The possible energy change is then of the order Γ . The multi-energy methods require a remarkable change in the phase of the propagation factor $\exp(ikr)$ due to a change of the $\boldsymbol{k}$ value. This is inaccessible by such a small energy variation as can be realized in the Mössbauer experiment. In this section, we propose a method, exploiting the fact, that the scattering phase itself is a rapidly varying function of the energy near the resonance. We will also discuss the experimental feasibility of this method.

The effect of the cancellation of the nuclear images for a system consisting of a reference nucleus and two scattering nuclei in positions $+\boldsymbol{a}$ and $-\boldsymbol{a}$ can be explained simply using arguments from Ref. 11. The function $U(\boldsymbol{r})$, representing the real-space image, is calculated for this system by substituting the value of the holographic oscillations due to the nuclei in positions $+\boldsymbol{a}$ and -$\boldsymbol{a}$, given by Eq. (17) into the Fourier holographic transform from Eq. (20). Then, the reconstructed real-space in the position $\boldsymbol{r}$ is given by:

$$
\begin{aligned}
U(\boldsymbol{r}) = \iint\limits_S \Big(& \frac{f_T(\boldsymbol{k},\, +\boldsymbol{a},\, E)^*}{a} e^{-ika}\, e^{i\boldsymbol{k}\cdot\boldsymbol{a}} \\
& + \frac{f_T(\boldsymbol{k},\, -\boldsymbol{a},\, E)^*}{a} e^{-ika}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{a}} \Big) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, d\sigma_{\hat{\boldsymbol{k}}} + c.c
\end{aligned}
\tag{24}
$$

The exponential factors oscillate, except for $\boldsymbol{r} = \pm\boldsymbol{a}$, and hence, the image function has maxima for $\boldsymbol{r} = \pm\boldsymbol{a}$. Consequently, the reconstructed image in the position $+\boldsymbol{a}$ is dominated by two terms:

$$
U(+\boldsymbol{a}) \;\simeq\; \frac{1}{a} e^{-ika} \iint\limits_S f(\boldsymbol{k},\, +\boldsymbol{a},\, E)^*\, d\sigma_{\hat{\boldsymbol{k}}} \;+\; \tfrac{1}{a} e^{ika} \iint\limits_S f(\boldsymbol{k},\, -\boldsymbol{a},\, E)\, d\sigma_{\hat{\boldsymbol{k}}}
\tag{25}
$$

where the first one corresponds to the real image while the second one leads to the non-physical twin image. From the properties of the effective scattering and absorption amplitude given by Eq. (18) and from the fact that the $F_M(\theta)$ is real and $F_M(\theta) = F_M(\pi - \theta)$ it follows that:

$$
U(+\boldsymbol{a}) \;\propto\; |f(E)| \left(e^{-ika} e^{-i\phi(E)} \;+\; e^{ika} e^{i\phi(E)} \right)
\tag{26}
$$

where $\phi(E)$ is the phase of the effective amplitude given by Eq. (18) . For a given energy ($\boldsymbol{k}$ vector value) the image function $U(+\boldsymbol{a})$ oscillates between real and imaginary values due to the propagation phase factors $\exp(\pm ika)$ and for some values of a equals zero. From Eq. (26) it is obvious that the condition for cancellation changes and depends on the value of the scattering amplitude phase factors $\exp(\pm i\phi(E))$. So, for example, the real space image obtained from a γ-ray hologram recorded in the sharp resonance and the image obtained from a single XFH hologram for the same energy will differ, because different pairs of atoms at $\pm\boldsymbol{a}$ could be affected by the cancellation. The Thomson scattering amplitude is almost pure real while the nuclear resonant scattering amplitude is pure imaginary.

When the Mössbauer effect is used for holography, the scattering phase can be changed directly by the de-tuning from the resonance. Of course, it is inevitably accompanied by a rapid fall-off of the resonant signal. If, however, two holograms would be taken for the two particular energy values $E = E_1$ and $E = E_2$, not too far from the resonance, the holographic transformation:

$$U^{'}(\boldsymbol{r}) \ = \ \sum_{E=E_{1,2}} \frac{U_E(\boldsymbol{r})}{f(E)^*} e^{ikr} \tag{27}$$

could remove the problem of the real and twin images cancellation. In Eq. (27) the $U_E(\boldsymbol{r})$ is a usual single holographic image obtained by the applying the holographic transform from Eq.(20) to the hologram recorded for a particular energy $E = E_1$ or $E = E_2$. The phase $\phi(E)$ of the scattering amplitude $f(E)$ depends strongly on the energy shift from the resonance. It is reasonable to take the two holograms symmetrically, on both sides of the resonance and denote $\phi(E_1) = \phi_1$ and $\phi(E_2) = \phi_2$. So, if for each of them the phase differs by $\pm\Delta 2$ from the phase at the sharp resonance $\phi(E_0) = \pi/2$, we can write that $\phi_1 = -\pi/2 - \Delta/2$ and $\phi_2 = -\pi/2 + \Delta/2$. Inserting the image functions $U_E(+\boldsymbol{a})$ recorded for the phase ϕ_1 and ϕ_2 to the proposed holographic transform (Eq. (27)) we get :

$$U^{'}(+a) \ = \ 2 - 2e^{2ika} \cos\Delta \tag{28}$$

and the reconstructed image intensity $|U(+a)|$ is proportional to:

$$|U^{'}(+a)| \ \propto \ \sqrt{1 + \cos^2\Delta - 2\cos(2ka)\cos\Delta} \tag{29}$$

If $\Delta = \pi/2$ then the oscillation of the reconstructed image intensity is completely removed for an arbitrary pair of nuclei at the positions $\pm\boldsymbol{a}$ relative to the reference nucleus. For realistic experiments the $\Delta = \pi/2$ condition is impossible to achieve and for holograms recorded for a smaller phase difference the oscillation can not be perfectly removed. This situation illustrates Fig. 9. The intensity oscillations of images for nucleus pairs at $\pm\boldsymbol{a}$ are plotted as a function of the $\boldsymbol{a}$ length for $\Delta = 0$ (single hologram, as in Fig. 5), $\Delta = \pi/2$ (idealized situation) and $\Delta = \pi/3$ (a realistic value used for the experiment simulation, corresponding to the de-tuning from resonance by $\pm 1.75\Gamma_{exp} = \pm 3.5\Gamma_s$. Apparently, the situation, which is experimentally possible, brings certain improvement. The oscillations are yet present but real and twin images never cancel. This fact has direct consequences for the reconstruction quality. Fig. 10 shows the real-space cuts obtained for $\Delta = \pi/2$ and $\Delta = \pi/3$. In the idealized case of $\Delta = \pi/2$ all nuclei are visible with almost equal intensity. For the experimentally realistic hologram recorded off resonance, the atomic scattering becomes also important, and because it is not taken into account in the reconstruction procedure, the real-space is distorted. In the realistic case, all nuclei are still visible but certain artifacts are present. Images of nuclei at the positions $\frac{3}{2}\,\frac{1}{2}\,\frac{1}{2}$ and the symmetry equivalent ones can be recognized, whereas in the image obtained from the single in-resonance hologram they were not present. In addition, the nearest neighbors are imaged with a stronger intensity as compared to the next nearest neighbors, as it could be expected from the spherical character of the scattered waves.

VII. CONCLUSIONS

We have presented the basic theory of the inverse γ-holography. The atomic resolution hologram is formed due the resonant nuclear scattering of the electromagnetic radiation. The acquisition is made by the resonance Mössbauer detection of the de-excitation products via the inelastic channel (conversion electrons). The absorbing and re emitting nuclei are microscopic holographic detectors. Due to a small size of nuclei, the character of the nuclear scattering process is almost ideal for holographic applications. The simulations performed in the frame of the SSC model proved however, that even for the idealized hologram spurious images and effects are observed in the real space reconstruction. They result from the overlapping of the real and twin images, typical for all kinds of single-energy holography. The polarization effects in the scattering and absorption are easy to remove by a modified holographic transform. We showed also explicitly the small role of the Thomson scattering in the hologram formation for the α-^{57}Fe structure. Despite the obvious limitations of the single energy γ-holography, the real space of the α-Fe structure could be reconstructed based on the experimental hologram. The hologram and the real-space image agree well with these resulting from the simulations. We proposed also a way how to eliminate the cancellation of twin and real images exploiting the strong dependence of the scattering phase on the energy, close to the resonance.

It becomes a challenge to use the most attractive property of the γ-holography with the resonance detection , namely its ability to image the magnetic structure with the hyperfine field resolution. The structure of magnetite (Fe_3O_4), in which Fe occupies two different crystallographic positions, is a well suited candidate. The magnetic hyperfine field for both sites differs enough to allow the hologram to be acquired separately for different Mössbauer transitions. However, it has to be noticed that for such a complicated system the hologram quality (statistics, the angular resolution and range) should to be considerably improved. In addition, it is expected that the hologram will be much more complicated due the increased role of the Thomson scattering and strong dynamical effects.

VIII. ACKNOWLEDGMENTS

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FIGURE CAPTIONS

Figure 1. (a) Magnetic hyperfine splitting of ^{57}Fe levels. (b) Geometry used for hologram calculation. The reference nucleus (hologram detector) is located at the origin, the scattering nucleus is at position $\boldsymbol{r}_i$. The angles θ_0 and θ_i are the angles between the magnetic field axis and incident and scattered photon propagation direction, respectively. The R stands for the reference wave, O for the object wave. The factors $F_M(\theta)$ describe polarization effects in scattering and absorption. (c) Spatial dependence of $F_M(\theta)$ for $M = \pm 1$ and $M = 0$ transitions, respectively (dark - low value, light - high value)

Figure 2. Holograms calculated for small cluster (radius 6.23Å) around the reference nucleus. (a,b) Pure nuclear holograms obtained for different transitions: $M = 1$ and $M = 0$. (c) Hologram resulting from the Thomson atomic scattering and subsequent $M = 1$ nuclear absorption. (d) Gabor-like hologram obtained for an isotropic scattering with a constant scattering phase shift $-\pi/2$. The multiplication factors refer to the maximum values from Fig. 1(c). The patterns are presented in the $\boldsymbol{k}$-vector scale in the full hemi-sphere. (dark - low intensity, light - high intensity).

Figure 3. The real-space images of the cluster structure obtained by applying the holographic transform to the $M = \pm 1$ hologram from Fig. 2(a). (a) The (001) cut in the plane of the reference nucleus. (b) The (001) cut 1.43Å (inter-planar spacing in the α-Fe structure) above the reference nucleus. (c) The (100) cut in distance 1.43Å from reference nucleus. The area of the imaged neighborhood is 14x14Å^2. Inverted gray scale (light - low intensity, dark - high intensity) is used for intensity, and no threshold value for elimination of weaker intensities is applied. The nodes of the square grid depict the lattice sites in the bcc structure.

Figure 4. Same as Fig. 3(a) but after a correction for polarization effects.

Figure 5. Intensity oscillation of the nuclear images at the positions $\pm\boldsymbol{a}$ due to the overlapping of the real and twin images. The distances of the nuclei, in the neighborhood of the reference nucleus for the α-Fe structure, are depicted by arrows.

Figure 6. (a) Hologram ($M = 1$ transition) for a small bcc cluster with a lattice constant a=3.02Å (to compare with Fig. 2(a)). (b) The resulting (001) real-space cut 1.43Å above the reference nucleus (to compare with Fig. 2(b)).

Figure 7. (a) Calculated and measured γ-ray holograms for the α-Fe structure. The patterns are presented in the $\boldsymbol{k}$-vector scale. (b) Profiles of the holographic oscillation for constant k_x values of 0Å^{-1} and 3.6Å^{-1} (points - experiment, lines - simulation).

Figure 8. Real-space images of the α-Fe structure obtained from holograms in Fig. 7(a). The real-space cuts calculated from simulation are shown in Figs 8(a)-(c), the cuts obtained from the measured hologram are depicted in Figs 8(d)-(f). The area of the imaged neighborhood is 14x14Å^2. Inverted gray scale (light - low intensity, dark - high intensity) is used for intensity, and no threshold value for elimination of weaker intensities is applied. The nodes of the grid depict the lattice sites in the bcc structure. The horizontal and vertical bars correspond to the spatial resolution resulting from the experimentally accessible $\boldsymbol{k}$-vector range for hologram acquisition.

Figure 9. Intensity oscillation of the nuclear images at position $\pm\boldsymbol{a}$ on applying the holographic transform from Eq. (25) to two holograms which differ in phase of the scattering amplitude by Δ. Dashed line corresponds to $\Delta = \pi/2$ (idealized situation), dotted line to $\Delta = \pi/3$ (simulation of real experiment) and solid line corresponds to $\Delta = 0$ (only one hologram at resonance and $\phi = -\pi/2$, as in Fig. 6). The distances of the nuclei, in the neighborhood of the reference nucleus for the α-Fe structure, are depicted by arrows.

Figure 10. The (001) cut of real space 1.43Å above the reference nucleus obtained by applying the modified holographic transform from Eq. (25) to two simulated holograms for $\Delta = \pi/2$ (a) and $\Delta = \pi/3$ (b)