Quantification of the neutron dark-field imaging signal in grating interferometry

C. Grünzweig,^{1,*} J. Kopecek,² B. Betz,¹ A. Kaestner,¹ K. Jefimovs,³ J. Kohlbrecher,¹ U. Gasser,¹ O. Bunk,¹ C. David,¹ E. Lehmann,¹ T. Donath,¹ and F. Pfeiffer⁴

¹*Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*

²*Institute of Physics ASCR, 182 21 Praha 8, Czech Republic*

³*Swiss Federal Laboratories for Material Science and Technology, CH-8600 Dübendorf EMPA, Switzerland*

⁴*Physics Department (E17), Technische Universität München, D-85748 Garching, Germany*

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Here we report on a mathematical description for the neutron dark-field image (DFI) contrast based on the influence of the thickness-dependent beam broadening caused by scattering interactions and multiple refraction in the sample. We conduct radiography experiments to verify that the DFI signal exponentially decays as a function of thickness for both magnetic and nonmagnetic materials. Here we introduce a material-dependent parameter, the so-called linear diffusion coefficient Ω . This allows us to perform a quantitative DFI-computed tomography. Additionally, we conduct correlative small-angle neutron-scattering experiments and validate the mathematical assumption that the angular broadening of the direct beam is proportional to the square root of the number of discrete layers.

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I. INTRODUCTION

Over the past years the neutron grating interferometry (nGI) technique^{1,2} was successfully established as a routine method in neutron imaging and is now used at different facilities.^{3–5} By the usage of the nGI technique information complementary to the conventional attenuation-based imaging, such as phase-contrast imaging¹ and dark-field imaging, is simultaneously obtained. Especially, the dark-field image modality gained rapidly in interest. Due to the magnetic moment of the neutron and hence its sensitivity to magnetic materials the dark-field contrast was used, on the one hand, to visualize bulk magnetic domain structures in two dimensions^{6,7} and even in three dimensions⁸ and, on the other hand, to visualize the magnetization processes.^{9,10} Dark-field contrast was also used to investigate structural inhomogeneities which are below the standard detector resolution and varying in the micrometer range.^{3,11} For both magnetic and nonmagnetic interactions the dark-field image (DFI) signal is related to small-angle/ultras-small-angle neutron scattering (SANS/USANS) and to multiple refraction in the sample caused by variations of either the nuclear or the magnetic interaction potential.

Quantitative neutron attenuation computed tomography (CT) has been known for decades and is based on the Beer-Lambert law, where the intensity decays exponentially as a function of the product of sample thickness and the material-dependent linear attenuation coefficient Σ . Tomographic investigations of USANS signals are reported in Ref. 12 using a double-crystal diffractometer device; however, no quantitative information is reported. Although DFI tomography investigations using the nGI setup are now routinely performed,^{3,8} a quantitative description, as for the attenuation-based CT, is still missing. Corresponding activities have been reported for x rays in the literature,^{13–16} but for neutrons, both the theoretical description and experimental verification are still missing. Both points are addressed in this paper.

II. SETUP AND PHASE-STEPPING ANALYSIS

A schematic depiction of the experimental setup used for the quantification of the DFI signal is shown in Fig. 1. In Fig. 1(a) the nGI interferometer setup is schematically shown, and it consists of a source grating G_0 , a phase grating G_1 , and an analyzer attenuation grating G_2 . The wedge-shaped sample is placed as close as possible to the front of the phase grating. The source grating G_0 (periodicity $p_0 = 1076 \mu\text{m}$) is an aperture mask with transmitting slits, placed in a monochromatic neutron beam with a wavelength of $\lambda = 4.1 \text{ \AA}$ and a wavelength spread of $\Delta\lambda/\lambda = 15\%$. It creates an array of periodically repeating line sources and effectively allows the use of relatively large, i.e., centimeter-sized, neutron sources without compromising the coherence requirements for the interferometer formed by G_1 and G_2 . The grating G_1 ($p_1 = 7.97 \mu\text{m}$), placed at a distance $l = 5.23 \text{ m}$ behind G_0 , acts as a phase mask and imprints periodic phase modulations onto the incoming wave field. Through the Talbot effect, the phase modulation is transformed into an intensity modulation in the plane of G_2 ($p_2 = 4 \mu\text{m}$), forming a linear periodic fringe pattern perpendicular to the optical axis and parallel to the lines of G_1 . For our setup, the periodicity of the fringe pattern is equal to $4 \mu\text{m}$. The absorption grating G_2 is placed at a distance $d_T = 19.7 \text{ mm}$ behind G_1 . The periodicity and orientation of G_2 is matched to the fringes created by G_1 . G_2 is placed in the detection plane, immediately in front of the detector. The fringe pattern is transformed to an intensity modulation by a linear movement of G_0 . Only the intensity modulation as a function of the position of G_0 is recorded at the detector with a spatial resolution of $100 \mu\text{m}$.¹⁷

Both the transmission image (TI) and the DFI were processed out of a series of nine images each taken with an exposure time of 10 s. The series of nine images corresponds to an equidistant stepping of G_0 over one period along the x direction perpendicular to the grating lines. Thereby the intensity signal $I(m, n, x_g)$ in each pixel (m, n) in the detector plane oscillates as shown in Fig. 1(b). To analyze these

FIG. 1. (Color online) (a) Schematic depiction of the experimental grating interferometer setup used for the nGI experiments. (b) Recorded intensity oscillation in one pixel if one grating is stepped horizontally over one grating period.

changes quantitatively, we write the intensity oscillation in each detector pixel (m, n) along the direction x_g in a Fourier series,

$$I_{m,n}^{s,r}(x_g) = a_0^{s,r}(m, n) + a_1^{s,r}(m, n) \cos\left(\frac{2\pi x_g}{p_2} + \phi_1^{s,r}(m, n)\right), \quad (1)$$

where a_0 is the averaged intensity, a_1 is the amplitude, p_2 is the period of the analyzer grating, and ϕ_1 is the transverse shift of the cosine-shaped intensity curve, with the assumption that higher-order terms are negligible. The superscripts refer to the data taken with sample (s) and reference (r) without sample. The normalized TI is calculated as

$$TI(m, n) = a_0^s(m, n)/a_0^r(m, n). \quad (2)$$

The visibility of the setup (without sample) is given by

$$V_r(m, n) = a_1^r(m, n)/a_0^r(m, n), \quad (3)$$

providing information about the maximum contrast of the interferometer. The DFI is calculated by normalizing the visibility with sample to the one without, leading to

$$DFI \equiv V(m, n) = \frac{V_s(m, n)}{V_r(m, n)} = \frac{a_1^s(m, n)a_0^r(m, n)}{a_0^s(m, n)a_1^r(m, n)}. \quad (4)$$

III. MATHEMATICAL MODEL TO DESCRIBE THE DFI SIGNAL

We now introduce a mathematical concept based on the influence of the width of the angular scattering distribution to describe the decay behavior of the DFI signal.^{13–15} Contrast in the DFI is obtained if a neutron beam transverses a sample that introduces an angular smearing of the incoming neutron beam due to SANS or USANS contributions for nonmagnetic or magnetic materials.

For one thin slice of a nonabsorbing material with a slice thickness Δt the angular scattering distribution after penetrating the material is assumed to have a Gaussian distribution, which can be written as

$$G_1(\theta) = \frac{1}{\sigma_1 \sqrt{2\pi}} \exp\left(-\frac{\theta^2}{2\sigma_1^2}\right), \quad (5)$$

with σ_1 being the width of the scattering distribution and θ being the scattering angle with respect to the direct beam direction. After penetrating N slices, under the assumption that all slices equally affect the angular spread and each new slice broadens the beam further, the final angular distribution is given by the convolution

$$G(\theta) = G_0(\theta) \otimes G_1(\theta) \otimes \dots \otimes G_N(\theta) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{\theta^2}{2\sigma^2}\right), \quad (6)$$

where the total scattering width σ is given by

$$\sigma = \sigma(N) = \sqrt{\sigma_0^2 + \sigma_1^2 + \dots + \sigma_N^2} = \sqrt{\sigma_0^2 + N\sigma_1^2}, \quad (7)$$

with σ_0 being the width of the direct beam. According to Eq. (1), the intensity recorded in each pixel can be written as

$$I_{m,n}^s(x) = I_{m,n}^r(x) \otimes G_{m,n}(x), \quad (8)$$

with the propagated angular distribution in the detection plane

$$G_{m,n}(x) = \frac{1}{\sigma_{m,n} d \sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma_{m,n}^2 d^2}\right) \quad (9)$$

at $d = x/\theta$ being the distance from the sample to the analyzer grating G_2 . Finally, the convolution leads to

$$I_{m,n}^s(x) = a_0^r(m, n) + a_1^r(m, n) \exp\left(-\frac{2\pi^2 \sigma_{m,n}^2 d^2}{p_2^2}\right) \times \cos\left(\frac{2\pi}{p_2} x - \phi_1(m, n)\right). \quad (10)$$

The influence of the total scattering width σ on the DFI is calculated from Eqs. (10) and (4) as

$$DFI = \exp\left(-\frac{2\pi^2 \sigma_{n,m}^2}{p_2^2} d^2\right). \quad (11)$$

From Eq. (11) we see, on the one hand, that the DFI signal exponentially decays as a function of the scattering width. On the other hand, we see that the DFI is most sensitive for scattering angles in the range of $\sigma \sim p_2/d$ as stated by the analytical description in Ref. 14. Large scattering angles lead rapidly to an unmeasurable DFI signal, and these neutrons will then contribute to the TI signal.

FIG. 2. (Color online) (a) TI and (b) of three step-wedged samples with $N = 10$ steps with a step thickness of 0.5 mm made of copper, brass, and brass containing 3 at. % lead. Averaged vertical profile data as a function step number N and corresponding exponential fits are shown for (c) the transmission signal $T(N)$ and (d) the visibility signal $V(N)$.

The angular scattering distribution $G(x)$ depends on the individual layer thickness Δt and the introduced beam broadening characterized by the scattering width σ of each layer.¹⁶ Here, we introduce a material-dependent parameter, the so-called *linear diffusion coefficient* Ω ,

$$\Omega \equiv \frac{\sigma^2}{\Delta t}, \quad (12)$$

providing the scattering width per unit length. Note that Ω is in analogy to the attenuation coefficient Σ for the conventional neutron attenuation imaging. The total scattering width along a certain beam path is hence given by

$$\sigma_{m,n}^2 = \int \Omega_{m,n}(t) dt. \quad (13)$$

Inserting Eq. (13) in Eq. (11) yields the DFI as

$$\text{DFI} = \exp\left(-\frac{2\pi^2 d^2}{p_2^2} \int \Omega_{m,n}(t) dt\right). \quad (14)$$

For a stack with a discrete number of identical slices N the DFI is given by

$$\text{DFI} = \exp\left(-\frac{2\pi^2}{p_2^2} N \Omega_{m,n,1} \Delta t\right), \quad (15)$$

with $\Omega_{m,n,1}$ being the material-dependent linear diffusion coefficient of one slice.

IV. THE LINEAR DIFFUSION COEFFICIENT Ω FOR NONMAGNETIC MATERIALS

For the validation of the mathematical description of the DFI signal in Eq. (15) we performed nGI experiments at the Swiss Spallation Neutron Source (SINQ) at the cold-neutron imaging facility ICON.¹⁸ Figure 2(a) shows the TI, and Fig. 2(b) shows the DFI of three wedge-shaped bulk samples. The first wedge is made of copper, and the other two wedges are made out brass, which is an alloy containing copper and zinc. One brass wedge additionally contains 3 at. % lead. For each wedge the thickness ranges from 0.5 to 5 mm in ten steps with an equidistant step thickness of 0.5 mm. Due to the similar attenuation coefficient Σ of the elements copper and zinc the three wedges can hardly be differentiated in the TI. As expected, the transmission signal $T(N)$ in Fig. 2(c) decays exponentially as a function of the number of steps N and is well described by the exponential decay fit function. In the DFI in Fig. 2(b) all three wedges are distinguishable, especially the two brass wedges. The visibility $V(N)$ as a function of steps N and the corresponding fits are shown in Fig. 2(d). For each

FIG. 3. (Color online) Grinding patterns obtained by optical light microscopy. (a) Copper as a one-phase material. The structure is due to the different lattice orientations of fcc grains. (b) Brass as a two-phase material. (c) Brass containing lead as a three-phase material. In (b) and (c) the grain structure is due to the different phases.

wedge an exponential decay behavior is obtained, confirming the validity of the mathematical model.

The experimental verification allows us to quantify our TI and DFI data. The linear attenuation coefficient Σ and the linear diffusion coefficient Ω according to Eq. (14) are given by

$$\int \Sigma(t) dt = -\ln T(t), \quad \int \Omega(t) dt = -\frac{p_2^2}{2\pi^2 d^2} \ln V(t),$$

with $p_2 = 4 \mu\text{m}$ and $d = 19.4 \text{ mm}$. We used a simple exponential decay function $y = A\exp(-Bx)$ to fit $T(N)$ and $V(N)$. This provides the material-dependent parameters: $\Sigma_{\text{Cu}} = (1.08 \pm 0.02) \text{ cm}^{-1}$, $\Sigma_{\text{Brass}} = (1.0 \pm 0.008) \text{ cm}^{-1}$, and $\Sigma_{\text{Brass,Pb}} = (0.96 \pm 0.004) \text{ cm}^{-1}$ and $\Omega_{\text{Cu}} = (0.62 \pm 0.03) \times 10^{-9} \text{ cm}^{-1}$, $\Omega_{\text{Brass}} = (1.42 \pm 0.03) \times 10^{-9} \text{ cm}^{-1}$, and $\Omega_{\text{Brass,(Pb)}} = (4.21 \pm 0.08) \times 10^{-9} \text{ cm}^{-1}$.

To clarify the different DFI signals of the wedges, in particular of the two brass wedges, we investigated the underlying metallurgy using optical light microscopy. Figure 3 shows the individual grinding surface patterns: In Fig. 3(a) copper as a one phase material shows a grain structure. The contrast in the DFI is due to scattering at these grain boundaries as the refractive index remains unchanged. In Fig. 3(b) the brass wedge shows two phases, the α phase with a chemical composition of $\alpha_{\text{Cu}} = 63 \text{ at. \%}$ and $\alpha_{\text{Zn}} = 37 \text{ at. \%}$ and the β phase with $\beta_{\text{Cu}} = 55 \text{ at. \%}$ and $\beta_{\text{Zn}} = 45 \text{ at. \%}$. The DFI contrast is due to the two phases which have slightly different refractive indices due their material composition. In Fig. 3(c) the second brass wedge contains 3 at. % lead, which forms precipitates as a third phase. The strong DFI contrast is due to the lead precipitates, which lead to strong discontinuities of the refractive index. The Pb precipitates are in a size and distribution range that causes the small- and ultrasmall-angle scattering to which the utilized nGI geometry is most sensitive.

V. QUANTITATIVE NEUTRON DFI TOMOGRAPHY RESULTS

The fact that the DFI signal dependence can now easily be described by Eq. (14) allows us to perform a quantitative DFI-CT experiment using the conventional filtered back-projection algorithm¹³ also used for the TI-CT reconstruction. The sample

as shown in the inset in Fig. 4(a) consist of two rods, a brass rod (containing 3 at. % Pb) and a copper rod. The reconstructed data¹⁹ are presented in Fig. 4. Horizontal and vertical slices from the TI-CT data are shown in Figs. 4(a) and 4(b), respectively. The corresponding slices of the DFI data set are displayed in Figs. 4(c) and 4(d). Both the Σ and Ω values are quantitatively reconstructed. Whereas for copper only the edges are visible in the DFI reconstruction due to edge refraction, for the brass rod both the interior and the edges show a contribution to the DFI.

VI. THE LINEAR DIFFUSION COEFFICIENT Ω FOR MAGNETIC MATERIALS

We extend our investigations to verify the validity of the exponential decay behavior of the visibility also for thin-layer samples of nonmagnetic and magnetic materials. These are, on the one hand, a paper stack with $N = 2, 4, \dots, 12, 14$ layers

FIG. 4. Quantitative DFI computed tomography of a phantom [see inset in (a)] made of copper and brass containing 3 at. % lead. (a) and (b) are reconstructions of Σ from the TI data set. (c) and (d) show reconstructions of Ω from the DFI data set.

FIG. 5. (Color online) TI, DFI, and averaged profile data with the corresponding exponential fits as a function of the number of layers for a paper stack with $N = 2, 4, \dots, 14$ layers with a layer thickness of $100 \mu\text{m}$ (left column) as a nonmagnetic material and a steel foil stack with $N = 1-10$ layers with a layer thickness of $10 \mu\text{m}$ (right column) as a magnetic material.

with a paper layer thickness of $100 \mu\text{m}$ and, on the other hand, two stacks of steel foil with $N = 1-5$ and $N = 6-10$ layers with a layer thickness of $10 \mu\text{m}$. The nGI results are shown in Fig. 5 for the paper stack on the left side and for the steel foil stacks on the right side. The paper stack is very visible in the TI in Fig. 5(a). The DFI in Fig. 5(b) shows a strong contrast as the paper consists of randomly oriented fibers in the micrometer range (compare scanning electron microscopy image in Fig. 6). The decay behavior of $T(N)$ and $V(N)$ as a function of the number of layers N is plotted in Fig. 5(c). From the fit parameters we obtain $\Sigma_{\text{paper}} = (2.01 \pm 0.03) \text{ cm}^{-1}$ and $\Omega_{\text{paper}} = (22.37 \pm 0.6) \times 10^{-9} \text{ cm}^{-1}$. For the steel foil stacks only the glue stripes to mount the stacks are visible in the TI in Fig. 5(d), and the corresponding plot of $T(N)$ in Fig. 5(f) shows basically a straight line. However, in the DFI in Fig. 5(e) both stacks are clearly visible. Already one layer is detectable, and for ten layers the DFI signal is saturated. Here, the DFI contrast is caused by the scattering of unpolarized neutrons at the domain walls.⁹ The plot of $V(N)$ as a function of layers N in Fig. 5(f) also shows an exponential decay behavior as for the nonmagnetic materials. Hence, we introduce a magnetic linear diffusion coefficient Ω_{mag} beside the nonmagnetic linear diffusion coefficient Ω . From the fit parameters we obtain $\Sigma_{\text{steel foil}} = (2.2 \pm 0.37) \text{ cm}^{-1}$ and $\Omega_{\text{steel foil}}^{\text{mag}} = (430 \pm 15) \times 10^{-9} \text{ cm}^{-1}$.

VII. CORRELATIVE SANS MEASUREMENTS

In the following we correlate the nGI data of the paper stack in Fig. 5 with SANS data^{20,21} to verify the assumption in Eq. (7) where the total angular beam broadening is given by the addition of the individual scattering width caused by each layer. The SANS data as presented in Fig. 5 show the direct beam and the patterns for an increasing number N of paper layers. The measured width σ_N after penetrating N layers of paper as given in Eq. (7) leads to the expression for the broadening caused by N layers:

$$\sigma_N = \sigma_1 \sqrt{N} = \sqrt{\sigma_{\text{measured}}^2(N) - \sigma_0^2}. \quad (16)$$

Here, the measured values of the beam broadening have been corrected for the width of the direct beam σ_0 . The validation of the assumption in Eq. (16) that the angular broadening of the direct beam is proportional to the square root of the number of layers is verified in the plot shown in Fig. 6.

VIII. CONCLUSION

In conclusion, we have found that the DFI signal decays exponentially as a function of thickness for nonmagnetic and magnetic materials. These results validate the introduced mathematical description of the DFI signal based on the

FIG. 6. (Color online) (left) SANS pattern (full detector size) of the direct beam and of the paper step wedge showing an increasing broadening for an increasing number of layers. (right) Evaluation of the Gaussian beam broadening as a function of layers. The σ_{measured} values are corrected to σ_0 (direct beam) and normalized to σ_1 to validate the square-root dependency $\sqrt{N}$ from Eq. (16).

reduction of the visibility due to sample scattering. We introduced a material-dependent magnetic and nonmagnetic linear diffusion coefficient Ω which is independent of the setup geometry, allowing us to conduct quantitative DFI-CT experiments. By conducting corresponding SANS experiments we quantitatively validate the theoretical assumption that the

angular Gaussian broadening of the beam is proportional to the square root of the number of layers and hence the thickness. We believe that the DFI quantification will further improve and establish this contrast modality as complementary information for nondestructive testing for objects with density variations below the detector resolution.

*christian.gruenzweig@psi.ch

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