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Edge Enhancement in Cold Neutron Imaging: A Comparison of Experiments at Edges and Interfaces with Ray-Tracing based on Refraction and Reflection.

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Abstract

In the past decade, increased neutron image resolution with digital detectors, approaching 10 μm, combined with more images obtained with cold neutrons, i.e., with neutrons having wavelengths longer than 3 Å, have yielded many examples of edge enhancement. Line profiles across an air-metal interface can show both reflection and refraction; in some samples, reflection can dominate while other samples show structure that is largely due to refraction. Thus far, evidence for Fresnel diffraction at sharp edges is lacking due to, as yet, insufficient detector resolution. With the exception of titanium, most common engineering metals have a neutron refractive index slightly less than one and application of geometrical optics such as Snell’s law and the Fresnel equations show that edge enhancement is detectable for low attenuation samples at about 4 Å and rapidly grows at longer wavelengths. Looking forward, imaging at a time-of-flight system could make use of the edge enhancement for sensitive detection of internal cracks and voids. Reduction, but not complete suppression, of edge enhancement is possible with close sample-to-detector distances. Edge enhancement effects have been shown to be determined by a number of parameters, both sample and beamline. As the range of samples grows, beamline performance increases, and the variety of imaging methods evolves, we should prepare for new examples of the edge enhancement effects as well as a change in the relative weights of reflection, refraction, and diffraction.

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Keywords: neutron imaging; edge effects; surface reflection; refraction; diffraction

1. Description of Edge Enhancement Effect

For many years, neutron radiography was done with thermal neutrons, mostly based on film techniques, until digital systems became the new standard in the 1990s. Surprisingly, no edge enhancements, such as the edge enhancement shown in Fig. 1, were reported. Instrument parameters that obscure the edge enhancement are low beam collimation, a short sample-to-detector distance, and the use of thermal neutrons. It is probable that a review of the film data will find more instances of edge enhancements and comments about the effect from skilled imagers of the early days of neutron radiography [1].
Figure 1 shows an edge enhancement effect at the air-steel interface of a diesel fuel injector, a representative sample from the field of engineering. The full explanation of the edge enhancement touches on many topics ranging from coherent neutron scattering cross sections, the index of refraction of a material, total surface scattering, and the wave-particle duality of slow neutrons. Herein, we strive to present a short, to-the-point discussion of the edge enhancement effect.

We follow the terminology of Goodman’s “Fourier Optics” [2]: Refraction is the bending of a neutron ray as it passes between regions of differing indices of refraction. Reflection has the property that the angle of reflection is equal to the angle of incidence. Diffraction is “any deviation of light rays from rectilinear paths which cannot be interpreted as reflection or refraction.” Examples of neutron refraction are compound optics [3, 4, 5, 6], polymer-based prisms [7], and metal wires [8]. Supermirrors are a recent example of neutron reflection, though detection of neutron reflection from surfaces of Be, graphite, Fe, Ni, Cu, and Zn was already reported by Fermi and Marshall in 1947 [9].

This wide-ranging definition of neutron diffraction includes both Bragg diffraction in crystalline materials [10] as well as the optical system in grating-based neutron phase contrast interferometry [11, 12, 13]. For the latter, the grating optics start with a G0 grating, a regular array of slits and absorber, essentially, an extension of the Young’s two-slit experiment. Towards the end of this paper, we will consider whether or not similar slit structures in engineering samples have the potential to generate a detectable interference pattern with today’s beam collimation and detector resolution.

Phase contrast imaging based on free-space propagation has been used for imaging lead objects [14, 15], a single crystal silicon block [15], aluminum foam [16], cracks in aluminum [17], iron cubes and cylinders [18], and aluminum castings [19]. The origin of the phase contrast images is now attributed to refraction; high transverse phase coherence is not easily achieved with pinhole neutron beam optics. Very recently, Treimer has theoretically examined diffraction of a coherent neutron beam in a glancing angle geometry with a metal surface and detected interference effects [20].

The NIST Center for Neutron Research (http://www.ncnr.nist.gov/resources/n-lengths/) tabulates neutron data such as total scattering and absorption cross sections, $\sigma_{\text{scat}}$ and $\sigma_{\text{abs}}$, and coherent scattering lengths, $b_{\text{coh}}$ [21]. The coherent scattering length is especially important for this work; it is usually measured with interferometric methods [22] and is largely constant over the range of cold and thermal neutron energies [23]. From these parameters, one can calculate the macroscopic scattering cross section, $\Sigma = N (\sigma_{\text{scat}} + \sigma_{\text{abs}})$; the refractive index, $n = 1 - \delta = 1 - N b_{\text{coh}} \lambda^2 / 2\pi$; and the critical angle for surface reflection, $\theta_{\text{crit}} = \lambda (N b_{\text{coh}} / \pi)^{1/2}$ [24, 25]. Fig. 2 shows the refractive indices and critical angles for many elements; a few elements were omitted to reduce overlap in the plots and the huge scattering cross section for gadolinium is off the scale of these plots.
Fig. 2. An overview of mass attenuation coefficients, the refractive index at 3 Å, and the critical angle for total surface reflection at 5 Å for selected elements at natural isotope abundance; alloys and compounds have coefficients, indices, and angles near the weighted average of the elements. Very few materials have a neutron refractive index greater than one, and therefore behave according to Snell’s law in the ways familiar to materials scientists accustomed to optical glass and visible light. For neutrons and most materials, we must adapt to the world of a refractive index less than one, particularly for imaging experiments with long wavelengths, $\lambda \gtrsim 3$ Å and high image resolution, $\lesssim 20$ μm.
2. Experimental Section

The samples studied consist of Al, Ti, Fe, steel, Cu, and Ni fabricated as thin foils, cylinders of various diameters, cubes, and plates. We note that Ti is commonly available both as pure Ti and as a Ti/Cu alloy. Some samples were polished by a machinist to an estimated surface smoothness of \( R_{\text{max}} \approx 0.5 \mu m \) and then cleaned with ethanol; other samples were used with a surface polish as received, perhaps an order of magnitude rougher; no significant differences were noted with either procedure. To definitively observe surface reflection, several supermirrors were studied. Layers of Ni and Ti are known to be suitable reflecting materials and are mounted on glass. We used small samples from Swiss Neutronics, \url{http://www.swissneutronics.ch/}, with \( m \)-values up to \( m=6 \).

Imaging was done at PSI ICON microtomography stage with polychromatic and velocity selected cold neutrons. Beam collimation ranged from \( L/D=300 \) to 600. An Andor CCD camera was used with \(^6\text{LiF}/\text{ZnS} 10 \mu m \) to 50 \( \mu m \) and GOS 20 \( \mu m \) scintillator screens; images were corrected with dark images and flat field images. Images were analyzed in either ImageJ or with routines written in Mathematica; plots were then made in either intensity units (ImageJ) or absorption units (Mathematica) with the former showing a more easily interpreted gain/loss count of neutrons in the edge enhancement and the latter presentation verifying the sample attenuation.

3. Reflection, Refraction, More Refraction, Ray-Tracing, and Diffraction

The following examples are representative of many experimental examples of edge effects. To give some order to the presentation, we will start with reflection. Then, we present refraction-dominated experimental results spanning different materials, sample geometries, and sample thicknesses. Two examples of ray-tracing are presented: first refraction only and then with the inclusion of reflection. We conclude with a hypothetical example of diffraction at a slit giving an intensity pattern which has not yet been observed in our experiments.

3.1. Total Reflection with a Neutron Supermirror

To examine the properties of total surface reflection in the geometry used for tomography, a supermirror on a glass support was examined, Fig. 3. The image from the CCD detector is shown in the inset and the trace represents intensity values from a line profile across the image. The supermirror is performing well under the tomography conditions and generates an intense and efficient reflection. The area of the peak labeled “reflection gain” is, to within 2%, the same as the peak area of “reflection loss”.

The glass support generates refraction peaks; one pair is observed on the left and are labeled “gain” and “loss”. Another pair of refraction peaks is believed to underlie the “reflection loss” peak.

![Image](image_url)

Fig. 3. An intensity plot and (inset) image of a supermirror slightly rotated with respect to the neutron beam. The dominant peaks are mirror attenuation and the two reflection peaks. “Gain” is used to indicate more neutrons at the detector than would be present in the flat field image or extrapolation from the air intensity values. The supermirror reflection gain and loss peaks are equal in area, to within 2%. The refraction loss peak is attenuated by the glass substrate.
3.2. Refraction at a Prism

At the start of this project, the very useful neutron ray tracing package McStas did not yet include refraction effects for the sample. Therefore, ray tracing of a simple plate was done with code written in Mathematica. To give a sense of the issues in ray tracing for edge enhancement analysis, let us consider a prism with an apex angle of 90°. For the geometry of Fig. 4a, the equations for a cubic prism are

\[ \sin \left( \frac{\pi}{4} + \alpha \right) = n \sin \left( \frac{\pi}{4} + \beta \right) \]  
\[ n \sin \left( \frac{\pi}{4} - \beta \right) = \sin \left( \frac{\pi}{4} - \gamma \right) \]  

where \( \alpha \) is the angle between the incident neutron and the direct line from the source to the detector and \( \gamma \) is the deviation angle of the exit neutron relative to the reference line, Fig. 4a. For Fe observed with \( \lambda = 3 \) Å, then \( n = 0.999989 \) and the deviation angle from the incident neutron ray is \( \gamma = 0.0013° \). For a sample-to-detector distance of 250 mm, this small deviation angle yields what seems to be minor, 5 \( \mu m \) shift at the detector plane. However, the cumulative effect of all neutrons along the prism face shifting to one side when convolved with the point-spread function of the imaging system contributes to the gain-loss peak pair experimentally observed, Fig. 4b, for the 45° orientation. A complete ray-trace analysis includes beam collimation, sample thickness, and the energy spread of the polychromatic neutron beam; a sketch of this analysis will be given in Section 3.6.

Fig. 4. A Snell’s law analysis of the origin of gain-loss peak for an Fe cube in the 45° orientation. The experimental intensity profiles were acquired with polychromatic cold neutrons observing the cube held 250 mm from the detector. The arrows indicate the direction of the neutron beam relative to the Fe cube.

As the Fe cube is rotated towards the 0° orientation (Fig. 4b), two other effects must be considered: the critical angle for total surface reflection and, for angles near the critical angle, the Fresnel equations defining the ratio of transmitted and reflected radiation [26]. In Fig. 4b, the Fe cube shows no sign of a surface reflection at 0°.

3.3. Refraction at a Prism, Cube, and Cylinder

The edge enhancement effect is observed for a variety of shapes: the Fe cube at 0°, the Fe cube at 45°, and an Fe cylinder, as shown in Fig. 5. To date, we have found no geometric structures made from Fe that fail to show the edge enhancement effect.
3.4. Effect of Material Thickness and Wavelength

Aluminum and steel were used to study the thickness dependence of the strength of the edge enhancement. It was found in previous measurements that Al layers of less than 1 mm do not provide significant edge effects. Therefore, plate type samples with thickness between 5 and 20 mm were placed perpendicular to the beam with the flat side surfaces in beam direction glancing to the beam of limited divergence (L/D=350) and profiles were taken close to the edges, Fig. 6.

At the first glance, it can be seen qualitatively that the edge effects increase directly with the sample thickness (or the possibly, the reflective area along the beam direction). In the same way, the pure attenuation signal from the main portion of the sample is attenuated as expected due to scattering and absorption. With the edge effect region, the loss and gain areas are correlated with sample thickness.

Five steel plates from a machinist’s blattlehre (feeler gauge) were imaged at three wavelengths and five sample-to-detector distances (SD). There is no detectable edge enhancement effect at 3.4 Å and SD=2 mm. The effect is largest
at 5.4 Å and SD=100 mm. Shown in Fig. 7a is the attenuation image, log(I₀/I), at 5.4 Å, SD=75 mm which shows a massive edge effect for the 600 μm thick steel plate, an easily seen effect for the 200 μm sample, and no discernible effect at 100 μm.

Quantification was done by selecting image regions, rotating to vertical, and performing column averages. The gain and loss edges were integrated and the area sums are plotted in Fig. 7b and also fitted to a quadratic function. The points roughly follow the expected trend for a \( \lambda^2 \) increase in refractive index, and thus an increase in the edge enhancement effect. The deviation seen for 600 μm at 5.4 Å in which the gain peak is smaller than expected may be due to the increase of neutron attenuation by steel at a Bragg edge (the velocity selector is known to have nearly a ±1 Å wavelength range across the field-of-view).

\[ \text{(a) image} \]
\[ \text{(b) fit} \]

Fig. 7. Edge areas for 200 μm (○), 300 μm (□), and 600 μm (●) and corresponding fits to a quadratic.

3.5. Effect of Beam Collimation and a Gedanken Experiment

Beam collimation studies have, so far, found nothing unusual, to an upper limit of L/D=650. At a constant sample-to-detector distance, the edge enhancement amplitude is steadily enhanced as the beam is better collimated.

In a Gedanken experiment, an aluminum plate was partly covered with gadolinium: Will the gain peak still be observed? A 20 mm Al plate was partially covered with a Gd absorber plate to prevent the direct access of the neutrons to the sample; the estimated precision of this attachment better than sub-millimeter. The sample was rotated around its vertical axis in 0.1° steps from -5° until +5° with respect to the beam direction. Fig. 8 shows the orientation judged to be best aligned with the beam.

A gain peak is observed for the portion of the sample covered by the Gd plate. Our arguments for neutron refraction cannot, if the Gd plate is perfectly aligned, explain the gain peak.

At this L/D, neutrons can certainly enter the side of the Al plate, but refraction in \( n < 1 \) material yields intensity behind the Gd absorber, not at the gain peak; in fact, some neutrons are detected behind the Gd plate at positions from 0.5 mm to 0.55 mm. To label the Gd/Al gain peak as due to a surface reflection is not logical as the amplitude is comparable to the gain peak observed for effects already labeled as refraction. Similarly, the onset of diffraction for Gd/Al sample with such a strong signal seems unlikely. Alas, it is mostly likely that sample alignment has proven to be exceedingly difficult with the sub-mm, fraction of a degree requirements of this Gedanken experiment.

3.6. Iron Prism: Ray-Tracing Example

Ray tracing was done in 2D based on Snell’s law for rays and omitting wave-like effects. The neutron source was simulated with 2000 positions evenly spaced across the pinhole and each position emitting 2000 neutrons evenly
Fig. 8. Comparison of the edge effects at a 20 mm thick Al plate partially covered with a Gd absorber plate (upper half of the sample). The bottom half of the Al plate is fully exposed to the neutron beam. Note the slight difference between the traces for the air portion of the image; the intensity difference is attributed to neutron scattering from the exposed Al sample.

distributed over ±half beam divergence = ± tan⁻¹ \left( \frac{\text{pinhole/2}}{beam length} \right); a gaussian intensity distribution was used, exp \left( \frac{-a^2}{2\text{half beam divergence}^2} \right). Thus, the paths of 4×10⁶ neutrons were examined in this Mathematica program. Mathematica encourages functional programming, possibly reducing the error rate in projects at the cost of slower computation, a few minutes for each simulation.

Fig. 9 shows the 2D geometry with angle definitions and four lines representing initial neutron propagation, refraction at front and back surfaces of the prism, and the detector, respectively. As each neutron was generated by the source and ray traced, its parameters were computed and stored in a list structure, about a 0.8 GB file. The parameter list included: \( y_0 \), neutron source position in the pinhole; \( \alpha \), neutron initial propagation angle; \( y_3 \), detector position in the absence of a sample, i.e., the intersection of line \( l_0 \) with line \( l_3 \); \( (x_1, y_1) \), the coordinates for the intersection of the neutron with the front surface of the prism, i.e., the intersection of line \( l_0 \) with line \( l_1 \); \( \beta \), the refraction angle at the front surface of the prism (see Eq. 1); \( (x_2, y_2) \), the coordinates for the intersection of the neutron with the back surface of the prism; attenuation within the prism based on the distance between \( (x_1, y_1) \) and \( (x_2, y_2) \) and a neutron attenuation of 0.2999 cm⁻¹; \( \gamma \), the refraction angle at the back surface of the prism (see Eq. 2); and \( y_3 \), the intersection of the neutron with the detector plane as represented by line \( l_3 \).

Shown in Fig. 10 are results of the ray-tracing simulations. Fig. 10a shows the intensity of the edge enhancement grows as the refractive index decreases; these simulations are for a pinhole diameter of 10 mm and a sample-to-detector distance of 250 mm. The estimated values for the refractive index and the attenuation in Fe are based on the parameters tabulated by NIST (http://www.ncnr.nist.gov/resources/n-lengths/) and the equations listed in Sec. 1. The thick line trace uses a refractive index estimated for Fe at 3 Å and an attenuation estimated for 2200 m/s,
corresponding to 1.789 Å. All traces show a transmission in air of unity (y>0) and a slightly curved trace due to the exponential increase in total attenuation within the prism (y<0). At a refractive index of unity, no edge enhancement effect is seen while as the refractive index is reduced, the edge enhancement grows. The “noise” in the traces is due to the limited number, $4 \times 10^6$, neutron rays used in each simulation; no smoothing functions have been applied to these results.

$$n/\text{Equal} 1$$

$$n/\text{Equal} 0.999989$$

$$n/\text{Equal} 0.999978$$

$$n/\text{Equal} 0.999967$$

$$\text{Minus} 1.5$$

$$\text{Minus} 1.0$$

$$\text{Minus} 0.5$$

$$0.0$$

$$0.5$$

$$1.0$$

$$1.5$$

$$0.7$$

$$0.8$$

$$0.9$$

$$1.0$$

$$1.1$$

$$1.2$$

$$1.3$$

$$1.4$$

$$y/\text{Slash} 1\text{mm}$$

transmission

(a) refractive index

$$D/\text{Equal} 10 \text{mm}, \text{SD} = 62.5 \text{mm}$$

$$D/\text{Equal} 10 \text{mm}, \text{SD} = 125 \text{mm}$$

$$D/\text{Equal} 10 \text{mm}, \text{SD} = 250 \text{mm}$$

$$D/\text{Equal} 5 \text{mm}, \text{SD} = 125 \text{mm}$$

$$D/\text{Equal} 5 \text{mm}, \text{SD} = 250 \text{mm}$$

(b) pinhole and sample-to-detector distance

Fig. 10. Ray-tracing results for an Fe prism with the geometry of Fig. 9. The thick traces are based on the experimental beamline settings and a refractive index for Fe estimated at 3 Å. The traces for other refractive indices and beamline settings are offset by steps of 0.1 transmission units. The shapes of the edge enhancement effects are strongly determined by the point spread function representing the incident neutron beam at the sample. The difference between the above simulations and the experimental trace, Fig. 4, indicates more broadening is needed in the simulation to match the experiment.

Fig. 10b shows the edge enhancement as a function of pinhole diameter and sample-to-detector distance. Briefly, large pinholes and short sample-to-detector distances will hide the effect and small pinholes and large sample-to-detector distances will amplify the effect.

3.7. Aluminum Plate: Glancing Angles and Ray Tracing

A 9.9 mm aluminum plate was imaged with 5.4 Å neutrons at glancing angles of ±3° in 0.04° steps and shows strong edge enhancement effects (Fig. 11a). At 9.9 mm thick, the aluminum sample is nearly transparent to the neutron beam passing entirely through the sample or refracted along the edge; integration of the edges labeled loss and gain show nearly equivalent areas at all glancing angles. The notch centered at zero degree glancing angle has an angular width of ±0.14°, similar to the ±0.167° of the neutron beam. At this wavelength, the predicted critical angle for aluminum metal is 0.252°. The polished aluminum surface has a surface roughness on the order of $R_{\text{max}} = 0.5 \mu m$. However, no surface reflection is detected at rotation angles from 0° to 0.25°. We note that the 0° set point is fitted with the assumption of a symmetric edge enhancement effect over the ±3°; the fitted set point is with 0.5° of the laser-aided sample alignment.

A ray-tracing program was written to model the attenuation, refraction, and reflection of neutrons at the edges of metal plates; diffraction effects were not included in the ray-trace model. Important equations are the approximation for the neutron refractive index, attenuation through the sample, Snells law, and the Fresnel equations for glancing angles (including the critical angle for total external reflection). The simulated sample was described with physical dimensions in 2D. The beamline is characterized with a beam divergence ($\pm tan[\text{pinhole diameter/source distance}]$), sample-to-detector distance, and detector pixel spacing. Ray-tracing begins, typically, with 1,000 point sources evenly spanning the width of the pinhole, and 1,000 angles evenly spanning the beam angular divergence. The fates of all $10^6$ neutrons are labeled with their calculated path, intersection with the detector, intensity at the detector (Fresnel equations), detector position and angle, and with and without the sample. Attenuation traces are calculated by $\ln(I_o/I)$, then digital noise is reduced by smoothing the traces with an n-point moving average. The Mathematica code was
parallelized yet still required a half-day for execution of a full angular range. The sinusoidal structure in the gain peak and the surface reflection is sampling noise; even with $10^6$ neutrons, the simulation is under-sampled.

All in all, the agreement between experiment and ray-tracing is considered good. For the refraction contribution, the ray-tracing reproduces the beam divergence feature centered at $0^\circ$ and the fall off of the edge effect towards $+3^\circ$. One notable disagreement between the two plots is the failure to detect in the experiment any sign of surface reflection. One possible explanation is that the beam divergence leads to a broad reflection and the relatively small surface area of the 9.9 mm thick plate gives a small reflection intensity.

3.8. Diffraction Effects

In the grating-based neutron interferometry experiment performed to acquire differential phase contrast images, the first grating is a based on the Talbot effect, a beautiful example of diffraction [2, 11, 12, 13]. This does lead to the question of when might a simple slit structure in the sample lead to an observable diffraction effect? Shown in Fig. 12 is a simulated Fresnel diffraction pattern as well as a blurred version of the pattern. With present-day neutron imaging having a geometric blur approaching 10 $\mu$m, the solid line shows the Fresnel diffraction effect may soon be observed.

4. Status

The experience gained on this project enables good prediction of when edge enhancement effects will generated by a sample as well as a estimate of the magnitude of the effect. For the examination of some engineering features such as cracks, this can be advantageous. Conversely, reduction of the edge enhancement effect for tomography projection data is also useful. Lacking, at this stage, is a facile mechanism for quantitative calculation of the effect. As noted earlier, McStas is a powerful and user friendly ray tracing tool, but lacks modeling of sample refraction. With an improved McStas or similar, it would be of considerable interest to model some of the experimental data collected in this project.

Does sample attenuation and refraction always fully account for the edge enhancement effect? For example, in none of our polished metal surfaces, excepting the supermirror, was surface reflection observed; yet, we note that Fermi and Marshall observed surface reflection from metals in 1947. That pioneering work had the advantages of a highly monochromatic neutron beam and a neutron counting detector. This suggests that surface reflections might be noted in engineering samples with increases in neutron energy resolution and detector dynamic range.

Next, when will Fresnel diffraction effects (see Fig. 12) be routinely observed? The steady improvements in beamline optics and detector performance indicate that day may be soon. As with refraction-based edge enhancement effects, the Fresnel effects can be advantageous for observing structural details.
In conclusion, edge enhancement effects have been shown to be determined by a number of parameters including sample, beamline, and the use of cold neutrons. As the range of samples grows, beamline performance increases, and the variety of imaging methods evolves, we should prepare for new examples of the edge enhancement effects as well as a change in the relative weights of reflection, refraction, and diffraction. This topic is well much an ongoing subject of study, particularly as one strives to maximize the quality of the neutron image.

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