FRACTAL APPROACH IN PETROLOGY: COMBINING ULTRA SMALL ANGLE (USANS) AND SMALL ANGLE NEUTRON SCATTERING (SANS)

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Fractal Approach in Petrology: Combining Ultra Small Angle (USANS), and Small Angle Neutron Scattering (SANS)


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Abstract. Ultra small angle neutron scattering instruments have recently covered the gap between the size resolution available with conventional intermediate angle neutron scattering and small angle neutron scattering instruments on one side and optical microscopy on the other side. Rocks showing fractal behavior in over two decades of momentum transfer and seven orders of magnitude of intensity are examined and fractal parameters are extracted from the combined USANS and SANS curves.

1. INTRODUCTION

Many natural processes and objects have been shown to be fractals. Examples include Brownian motion, thermal convection, earthquakes, snowflakes, coastlines, rivers, faulting, folding and volcanic eruptions. Petrology is a branch of science that deals with the origin and evolution of rocks. So, its purpose is to study changes that occur naturally in rocky complexes, namely, sediments which undergo physical and chemical alterations, magmatic fluids which solidify, rocks which undergo partial or total melting. Fractal geometry is the natural mathematical language to describe much of what petrologists observe. Fractal geometry does not describe the mechanism that produces the fractal scaling, but it nonetheless helps to sort out possible mechanisms or explanations. Although much has been accomplished in quantifying rock and mineral chemistry, comparatively little effort has been made to quantify texture. Recent progress in ultra-small angle neutron (USANS) and X-ray scattering (USAXS) instrumentations enables one to access the microstructure of rocks well beyond the limit of SANS instruments. In this paper we present new USANS, and SANS experiments performed on various samples.

2. THEORETICAL BACKGROUND

A particularly fortunate situation arises when rocks are investigated by means of neutron scattering. In this case the system, even if strictly multi-phase, can be treated as a two-phase system as most of the scattering originates from the contrast between the inorganic components and the voids. When a beam of neutrons illuminates a volume V in which scattering centers are distributed according to a distribution law $\rho(r)$, scattering events take place and a diffused beam will be generated, whose differential scattering amplitude $dA(Q)/dV$ as a function of the scattering variable $Q$ will be given by
\[ \frac{dA(Q)}{dV} = \rho(r) \exp(-iQr) \]  

In integrated form, equation (1) relates the scattering amplitude \( A(Q) \) to the Fourier transform of the scattering length \( (Q=4\pi \lambda^{-1} \sin \theta, 2\theta \) being the scattering angle and \( \lambda \) the wavelength of neutrons).

In the late eighties there has been a strong interest to describe the scattering from natural systems (in primis rocks) in terms of fractal structures (mass and/or surface fractals). However, these attempts led to limits in the interpretation of data because most of the power law exponents found were in a range of uncertain attribution, and also because the \( Q \) range in which data could be obtained was too limited (often less than 1.5 decades). To extend the \( Q \) range we have modified the Oak Ridge National Laboratory USANS camera, which now incorporates the suggestions to suppress the wing effect by using two triple bounce channel cut ideal crystals in the Bonse-Hart set-up¹, and we have measured again some of the samples run earlier. In a few cases we have also extended the high \( Q \) portion of the scattering by performing our experiments at the TOF SANS instrument at the Rutherford Appleton Laboratory (UK), and by making use also of the high \( Q \) detector bank. By doing so we have been able to span almost seven decades of momentum transfer.

3. EXPERIMENTAL

The SANS and IANS results have been obtained at the ISIS pulsed neutron source of the EPSRC Rutherford Appleton Laboratory (UK) using the "LOQ" spectrometer² and at the Oak Ridge National Laboratory using the 30m SANS camera. Details of technical and experimental aspects together with data reduction procedures are given elsewhere¹,³.

The USANS results have been obtained at the HFIR USANS facility of the Oak Ridge National Laboratory USA. Details of technical and experimental aspects together with data
reduction procedures are given elsewhere\textsuperscript{1}. As the USANS camera becomes unreliable for \( Q > 0.003 \), there is a small region of \( Q \) not covered by both USANS and LOQ instruments.

4. DATA ANALYSIS

We shall now present the scattering equation for mass fractals and for surface fractals. Bale and Schmidt\textsuperscript{4} derived an expression for the correlation function of perfect surface fractals, i.e. fractals whose surface is self-affine and whose surface roughness scales according to a power law of the kind \( S(r) = S_{0} \left( r/l_{\max}\right)^{-2-D_{s}} \), where \( l_{\max} \) is the upper limit for the scale invariance (i.e. the largest size for which the surface is still a fractal). In terms of the surface fractal dimension \( D_{s} \), the scattering function \( I(Q) \) has been derived by Mildner and Hall\textsuperscript{5}:

\[
I(Q) = Q^{-1} \Gamma(\beta) l_{\max}^{-\beta}[1+(Q l_{\max})^{-2}]^{-\beta/2} \sin((D_{s}-1) \arctan(Q l_{\max})) \text{, where } \beta = 5-D_{s}. \tag{2}
\]

When \( l_{\max} \gg 1/Q \) (i.e. in the range of linearity in a log \( I(Q) \) vs. log \( Q \) plot) we have a power law dependence of \( I(Q) \) from \( Q \) with exponent \( \beta+1 \). The existence of a lower limit for the scale invariance, \( l_{\min} \), is indicated in a double log plot by a flattening of the scattering curve at high \( Q \) values, following the linear portion. Fig. 1 shows the USANS result obtained for a sample of rock (benmoreitic inclusion in hyaloclastite, Linosa Island, Italy). Symbols indicate slit smeared and point desmeared experimental intensities, while the line indicates fit to the above scattering equation for surface fractals with a fractal dimension \( D_{s} = 2.3 \) and a cut-off dimension \( l_{\max} \) of \( 3.9 \times 10^{3} \) Å. An entirely analogous equation can be derived\textsuperscript{6} for mass fractals:

\[
I(Q) = Q^{-1} \Gamma(\beta) l_{\max}^{-\beta}[1+(Q l_{\max})^{-2}]^{-\beta/2} \sin((\beta-1) \arctan(Q l_{\max})) \text{, where } \beta = D_{m}-1. \tag{4}
\]

where \( D_{m} \) is the mass fractal dimension and \( \beta = D_{m}-1 \). Also in this case the scattering equation in the range of linearity in a log \( I(Q) \) vs. log \( Q \) plot gives a power law with exponent \( \beta+1 \).

5. RESULTS AND CONCLUSION

Figure 2 shows USANS, SANS+IANS data for the same rock shown in figure 1. The rock shows fractal behavior in slight more than two order of magnitude in \( Q \) (and therefore in length scale) and seven orders of magnitude in intensity. Diffraction peaks are barely shown in the highest region of scattering variable \( Q \), where the flattening of
the scattering curve is due to $l_{\min}$, while the flattening in the small Q region is due to the cut-off distance $l_{\max}$.

Figure 3 shows combined USANS, SANS and IANS data for a sedimentary rock for which the best fits were obtained with the mass fractal equation. Fits yield a fractal dimension $D_m = 2.85$ and a cut-off distance $l_{\max}$ of $6.0 \times 10^3$ Å. The rock shows fractal structure in slight less than three orders of magnitude in Q (and therefore in length scale), while intensity varies about eight orders of magnitude.

Figure 4 shows the transition from a surface fractal structure to a mass fractal structure. The sample is a dinosaur bone. Symbols are point geometry USANS and SANS data. Lines are fits to equation 2 and equation 3 of the text. Data are well reproduced except in the transition region from surface to mass fractals.

In conclusion, examples of rocks showing mass and surface fractal geometry have been shown. These indicate the importance of combining USANS and SANS data to extend the range of momentum transfer explored.

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