

FRACTALS IN MATERIALS RESEARCH

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ABSTRACT

The Richardson-Mandelbrot (R-M) fractal equation for lines (profiles and perimeters), and the Hack-Mandelbrot (H-M) fractal equation for perimeters and areas (lakes and islands) are examined closely in terms of the original derivations and assumptions. Of concern is the implicit assumption that theoretical results obtained for special geometrical figures also apply automatically to natural irregular curves. Discrepancies are found in the dimensionality of the equations, predictions of an infinite line length in the fractal plot, and lack of provisions to obtain a "true" line length. The fractal dimension D is not defined in physical terms. A serious limitation to the H-M expression is the requirement of constant island shape. The lack of commonality between the two fractal equations is most disturbing.

Inconsistencies also arise between the theoretical predictions and the experimental findings. We observe nonlinear fractal plots and variable values of D , conflicting results for islands and lakes, and different results from vertical and horizontal sections.

Solutions to some of these problems are proposed. The dimensionality shortcomings in the R-M and H-M equations are corrected, a linearization treatment is outlined for the reversed sigmoidal curves of materials fractal plots, an alternative equation is proposed that eliminates the restriction on island shapes, and suggestions are made to combine the two fractal equations of R-M and H-M into one.

Key words: fractals, Hack-Mandelbrot, reverse sigmoidal fractal curves, Richardson-Mandelbrot, Tomkeieff.

INTRODUCTION

Research on the fractal behavior of nonplanar surfaces and their traces is proceeding rapidly and in many different ways. There is also a major lack of agreement among the principal theories and experimental methods employed. Furthermore, conflicting results are frequently reported, and interpretations are often confounded by insufficient or limited data (Feder 1988). Consequently, the results obtained by different means are difficult to interpret and compare.

Fortunately, studies to correct the problems attendant to materials fractal research are underway. A more rational and self-consistent methodology for treating the fractal properties of materials is slowly being achieved, and these findings are expected

to promote uniform interpretation of results for a wide range of materials.

Our approach in this paper is to examine closely the stated postulates and assumptions in the two fractal equations, then to assess the extent of agreement between the theoretical predictions and the experimental results. Proposals are then put forward to rectify the discrepancies noted.

THEORETICAL BACKGROUND

Both the Richardson-Mandelbrot (R-M) and Hack-Mandelbrot (H-M) fractal relationships were developed from simple mathematical or geometric models. The experimental fractal data available at that time were minimal. The Richardson equation (Mandelbrot 1977, 1982) expresses the rate of increase of the length of coastlines (or irregular planar curves). "This exact formula..." is

$$L(\eta) = \eta^{1-D} \quad (1)$$

where $L(\eta)$ is the apparent length of an irregular planar curve, which varies as a function of η (or ϵ); i.e., the length of the measuring 'yardstick' used to approximate the length of the irregular curve. D , the fractal dimension, is related to the slope of the linear form of Eq. (1), which is

$$\log L(\eta) = (1 - D) \log \eta \quad (2)$$

The slope $m = 1 - D$. D is a constant, and can have fractional values between 1 and 2. When $\log L(\eta)$ is plotted vs $\log \eta$, Eq. (2) predicts a straight line that extends without limit in either direction.

In order for Eq. (1) to be valid, the irregular curve must possess the property of "self-similitude"; i.e., the curve should have the same apparent visual shape and configuration at all magnifications. As Mandelbrot (1982) puts it, "In order for the exponent of self-similarity (D) to have formal meaning, the sole requirement is that the shape be self-similar, i.e., that the whole may be split up into N parts, obtainable from it by a similarity of ratio r ."

Thus, the major requirements of a fractal plot are (1) that it is linear, (2) that it extends without limit in either direction, and (3) that the slope, and thus D , is constant over the entire fractal plot. If these conditions are not met, then the validity of the self-similitude assumption is in doubt, and fractal behavior is questionable.

The other major fractal relationship being used in materials research is due to H-M. It relates the perimeter length L of a closed planar loop (or 'island') to its area, A . (Note that Eq. (1) does not contain an area term.) Mandelbrot (1977, 1982) invokes a "standard equation of Euclidean geometry"

$$L = K A^{1/2} \quad (3)$$

where the constant K is a number entirely determined "for each family of standard planar shapes (closed loops) that are geometrically similar and have different linear extents". Thus, a log-log

plot of L vs A yields a family of parallel lines of slope $1/2$, but with different intercepts determined by the particular planar shape being considered. Mandelbrot (1982) then modifies Eq. (3) by postulating that the L term behaves fractally whereas the A factor does not. This gives

$$A = K_S L^{2/D} \quad (4)$$

The shape coefficient K_S has a constant (numerical) value for any one set of geometrically similar islands. Different values of K_S are required for sets of islands having other shapes. Note that Eq.(4) does not explicitly provide for a variable measuring yardstick η , as in Eq. (1).

The major requirements for the validity of Eq. (4) are that (1) all islands should have the same shape, (2) a log-log plot of A vs L should yield a straight line that extends without limit in either direction, and (3) D should have a constant value.

DISCREPANCIES WHEN APPLIED TO MATERIALS SYSTEMS

The principal characteristics, assumptions and implied consequences of the R-M and H-M fractal relationships have been outlined above. Several theoretical discrepancies are apparent from the discussion. Moreover, we find consistent deviations from the theoretical predictions when applied to materials research results. We will point these problems out briefly here, then in the next section propose practical solutions.

Referring to Eq. (1), we see that it is dimensionally incorrect, except when $D = 0$. Several ways have been proposed to rectify this situation and some of the more promising approaches will be presented later.

Another drawback to Eq.(1) is the failure to provide for a "true" length for the irregular curve. A "true" value for a fixed (nonfractal) curve would correspond to the length of the curve as $\eta \rightarrow 0$. The length of a fractal curve, however, is expected to approach infinity as $\eta \rightarrow 0$. In order to obtain a fixed value for the length of the curve, arbitrary values of η have been selected by various researchers. This procedure is subjective and unsatisfactory.

A clearcut physical definition of the meaning of the fractal dimension D is missing. Attempts have been made to clarify this unclear situation, and will be discussed in the next section.

A major discrepancy arises with the fractal plots of irregular planar curves such as fracture profiles. Instead of a straight line extending without limit in both directions, the fractal plot is curved. Asymptotes tending to zero slope appear at large and small values of η . Thus there is a smoothly bending curve, the reverse of the "sigmoidal" kinetic reaction curves of chemistry (Underwood, 1991). These so-called reverse sigmoidal curves (RSC), or segments thereof, occur without exception in fractal plots of natural irregular curves. If the investigated range of η is too small, all that is observed is a segment of the RSC (Rigaut, 1990).

This nonlinear behavior in the fractal plot is *a priori* evidence that self-similarity does not exist, and that the curve is not fractal. However, this evidence is blandly dismissed or ignored, and cutoff values are designated to exclude those portions

of the fractal curve that inconveniently do not conform to prior theory. And merely by drawing a straight line through the curved fractal plot does not constitute convincing evidence of fractal behavior.

Similar objections to those listed above can be raised against the H-M relationship. There are dimensionality problems, a lack of linearity in the fractal plot, and a requirement for constant island shape. Inspection of Eq. (4) reveals that its dimensionality is not correct, except for $D = 1$. A possible way to circumvent this deficiency is proposed later. Another problem with Eq.(4) is the requirement that all islands must have the same shape. Moreover if serial sectioning is employed, the shape must remain constant from section to section. It is highly unlikely that the shapes of the islands from an irregular fracture surface conform to this condition. We also find, contrary to the predictions of Eq.(4), that the plot of $\log A$ vs $\log L$ is not linear indefinitely. In fact, data from a series of Koch snowflakes demonstrate this immediately because the area curve converges to a constant value while the perimeter length proceeds to infinity.

Again, we find that much of the published data that claim linearity in the fractal plot can only do so because of the limited range in perimeter length (and perhaps because only one island is followed from section to section!) Feder (1988) also questions the validity of D determined from insufficient data.

RECONCILIATION OF DISCREPANCIES

Several proposals have been advanced to correct the dimensional inequalities in Eqs. (1) and (4) (Huang, et al. 1990). One way to make Eq.(1) dimensionally correct (Underwood, 1985) is to substitute a dimensionless ratio for η , according to

$$L(\eta) = L_0 (\eta/\eta_0)^{1-D} \quad (5)$$

where η_0 is an arbitrary constant with dimensions of length; its magnitude does not affect the slope of the fractal plot. This equation satisfies the dimensional requirements and, in general, $L(\eta)$ is proportional to L_0 . When $\eta = \eta_0$ or $D = 1$, $L(\eta) = L_0$.

Similar manipulations of Eq.(4) to make it dimensionally correct give

$$A = A_0 (L_p/L_0)^{2/D} \quad (6)$$

where L_0 is an arbitrary length constant and A_0 has dimensions of length squared. The slope of the log-log plot of A vs L_p is not affected by the magnitude of L_0 nor is the value of D changed by these normalizing constants. However, since A tends to a constant value while L_p increases indefinitely, in the limit we would anticipate that $D \rightarrow \infty$.

The fractal dimension in Eqs. (4) and (6) applies to the perimeter of the loops or islands. Mandelbrot's original treatment clearly reveals he is dealing with a two-dimensional figure. Thus, later attempts to assign a fractal dimension of $(D-1)$ to the perimeter lengths are questionable (Mecholsky, et al., 1989). Moreover, Feder (1988) believes the exponent should be D , and not $2/D$.

Theoretical definitions of 'fractal' and 'fractal dimension' have been a subject for much speculation. Mandelbrot has recently

proposed a new definition (Feder, 1988): "A fractal is a shape made of parts similar to the whole in some way." For a fractal Brownian function, Feder (1988) lists the attributes, both self-similar and affine, of five different D's. The physical meaning of D is also unclear. An indirect way to describe its characteristics is by comparison with other parameters that have simple physical meanings. In one study (Underwood and Banerji, 1986), a close similarity between plots of D and three dimensionless roughness parameters R_p , R_L and R_S vs fracture surface configuration was demonstrated. R_p is sensitive to the local shape of the curve, while R_L and R_S can increase either by increased tortuosity or by higher peaks. Thus, it appears that the attributes of shape, roughness and local configuration of a curve are factors that influence D.

Perhaps the most important problem with the fractal treatments of profiles and slit islands is the lack of interconsistency between the R-M and H-M theoretical treatments. Most experimental results are also widely divergent. On the one hand, Eq.(1) (or Eq.(5)) applies to open or closed profiles and the variables are curve length and yardstick length. Area does not appear in their formulation. A vertical section is generally used to generate the profile. On the other hand, Eq.(4) (or Eq.(6)) applies only to closed loops and the variables are area and perimeter length. η does not appear explicitly in this equation. A horizontal section (or sections) is generally employed to generate the islands (or lakes).

In spite of these differences, both methods depend on sections cut through a nonplanar surface. A planar section, regardless of its angular position, should relate geometrically to that surface. Basically, if any irregular surface of any configuration is cut by a planar section, the ensuing trace should be related to the surface from which it came. Thus, it does not matter, in principal, if the section plane is 'vertical' or 'horizontal' or in between. The general stereological equations relating surfaces and their traces are still valid (Underwood, 1970). Geometrically speaking, the R-M and H-M relationships must be related. So it is not unreasonable to expect that an underlying relationship exists between these two methods.

What is desired is an expression that combines both Eqs.(5) and (6) and retains the three variables: A, L_p and η . One of the more promising relationships appears as

$$L_p/L_0 = (A/A_0)^{D/2}(\eta/\eta_0)^{1-D} \quad (7)$$

A similar expression, used in another connection, has been found in Feder (1988). Under the appropriate conditions, Eq. (7) yields either Eq.(5) or (6). If a profile is under investigation, the area term is held constant and we have

$$\log(L_p/L_0) = \log K' + (1-D)\log(\eta/\eta_0) \quad (8)$$

which is comparable to Eq. (5). If islands are being studied with constant η , we can write

$$\log(A/A_0) = \log K + (2/D)\log(L_p/L_0) \quad (9)$$

and this gives the same value of D as Eq. (6). The shape restriction noted previously for Eq.(6) still applies; however, it can be

circumvented by a different approach.

Using the assumption-free equations of stereology, the H-M fractal relationship can be generalized to be independent of the shape restriction. An appropriate equation for planar loops of any configuration was published without proof by Tomkeleff (1945). The two-dimensional form (Underwood, 1970) is

$$A = \bar{L}_2 L_p / \pi \quad (10)$$

where A and L_p are as before, and \bar{L}_2 is the island mean intercept length. Comparison with Eq.(4) reveals that the quantity (\bar{L}_2/π) is akin to the shape coefficient. In Eq.(10), however, there are no restrictions on the shape of the islands. Unfortunately, \bar{L}_2 is not constant and should be expected to vary with island size and shape. For example, \bar{L}_2 decreases from 0.45 to 0.17 for the first six figures in the Koch snowflake series. Thus, Eq. (10) has three variables to cope with.

An alternative way to present Eq.(10) is to combine factors as indicated by

$$\log(A/\bar{L}_2) = \log(1/\pi) + \log L_p \quad (11)$$

which predicts a straight line of unit slope for closed loops of any shape. A plot of Eq.(11) for the first six Koch snowflake figures confirms this linear behavior nicely. A fractal version of Eq.(11) that parallels Eq.(6) can be written

$$A/\bar{L}_2 = K_L (L_p/L_0)^{1/D} \quad (12)$$

where K_L and L_0 are constants with dimensions of length. Now, if loops with irregular perimeters possess fractal characteristics, the slope will equal $1/D$ and not unity (as in Eq. (11)). The values of \bar{L}_2 can be obtained for individual islands by image analysis, or else Eq.(10) can be used. In some cases, an average value of \bar{L}_2 for all islands may prove feasible. If required, η may be introduced into Eq. (12) as in Eq.(7).

The requirement for a "true" length or "true" surface area crops up frequently in the literature. At the same time, there is a need for an objective way to linearize the fractal plot, and thus obtain a constant value of D . A procedure that accomplishes all these objectives is available in a general method that linearizes RSCs (Underwood, 1991; Underwood and Banerji, 1986). The equation can be written for profiles as

$$\log \frac{R_L(0) - R_L(\infty)}{R_L(\eta) - R_L(\infty)} = K \eta^{D_\beta - 1} \quad (13)$$

Where D_β is the modified (constant) fractal dimension. The profile (or linear) roughness parameter R_L is defined as the profile length divided by its projected length. $R_L(\eta)$ is the only variable term in the LHS of Eq. (13), so we can write in functional form

$$f(R_L(\eta)) = K \eta^{D_\beta - 1} \quad (14)$$

The similarity of Eq. (14) compared to Eq.(5) is apparent. Plots of experimental data according to Eq. (13) give excellent straight

lines, over a range in η of less than 1 μm to over 400 μm . Thus, we obtain both linearity of the entire fractal plot and a constant slope, which leads to a constant (modified) fractal dimension. Moreover, the "true" length is forthcoming immediately from $R_L(0)$, a constant whose value is determined as $\eta \rightarrow 0$. Although $R_L(0)$ cannot be measured experimentally, it can be determined unambiguously from the experimental fractal data (Banerji, 1987).

DISCUSSION

The original formulations of Richardson-Mandelbrot and Hack-Mandelbrot for profiles and closed loops show many discrepancies. It has been possible to rectify most of them, including dimensional discrepancies in the equations, constancy of island shape restrictions, nonconstant value of D , nonlinear fractal plot, and lack of provision for a "true" curve length. Some indications of the physical meaning of D have emerged.

Interpretations of the experimental data have suffered from a tendency to make subjective decisions. In this regard, straight lines are frequently drawn through curved portions of the fractal plot, ostensibly to obtain a local fractal dimension. The actual data do not always support these *ad hoc* decisions. Another common mistake is to relate a certain range in η (from the fractal plot) to a size range of microstructural features (such as particle spacings) in the fracture surface (Dauskardt RH et al., 1990). This procedure is incorrect because each point on the fractal curve comes from the entire apparent curve length, and cannot be related to features that occupy only portions of the profile length.

Even more important than the detailed inconsistencies of the R-M and H-M relationships is the lack of agreement between these two methods. Procedures for unifying the two fractal equations are proposed. One approach combines the two original expressions into one equation with three variables: A , L_p and η , according to

$$L_p/L_0 = (A/A_0)^{D/2} (\eta/\eta_0)^{1-D} \quad (7)$$

This expression still retains the original requirement for constant island shape. A method that avoids the shape restrictions of H-M invokes the fractal form of Tomkeieff's stereological equation for closed planar figures

$$A/\bar{L}_2 = K_L (L_p/L_0)^{1/D} \quad (12)$$

This equation contains no shape restrictions.

Another important inference about the irregular curves of nature can be drawn from the evidence presented above, and is based on the breakdown of the prediction of linearity in the fractal curve. Fractal plots that have the RSC shape, that exhibit asymptotic behavior as $\eta \rightarrow 0$, and that have a constant "true" length must derive from fixed curves, rather than fractal curves. The basic requirement of self-similarity is lacking, so as the measuring unit gets smaller and smaller, the length of the fixed curve must converge to a constant value. As Falconer (1990) puts it, "There are no true fractals in nature."

CONCLUSIONS

(1) An irregular natural curve cannot be deemed fractal until it is demonstrated to be fractal. One of the best ways to check for "self-similitude" is through the linearity of the entire fractal plot.

(2) The usual fractal plots of nature have a reverse sigmoidal shape. This behavior is opposed to the straight lines obtained by mathematical models or special geometric figures.

(3) Any sectioning plane, regardless of its angle or position, that cuts an irregular surface, should be stereologically related to that surface. This applies regardless of whether sections are horizontal, vertical or intermediate, and whether profiles, loops or intermediate configurations are generated.

(4) The irregular curves of nature are not fractal but are curves of fixed configurations. Thus, as the decreasing magnitude of the measuring unit η approaches the magnitude of the smallest segments of the fixed curve, the length of the curve must converge to a fixed value.

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