Quantitative Comparison of Lineal Analysis to Box Counting Analysis of a Real Microstructure

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Summary – Expressions relating box counting and lineal analysis are developed. Both methods are used for fitting the spacing distribution of a real microstructure. The relation to grain size distribution is discussed.

1. Conversion of HarFA spectrum into an Areal Size Distribution.

HarFA (Harmonic Fractal Analyzer) will generate a plot of the fractal dimension D vs. the ln(s) where s is the box size. The fractal dimension is defined as

$$D(s) = -\,\mathrm{dln}(N)/\mathrm{dln}(s),$$

where N is the number of boxes that contain a black pixel when a grid of size s is overlayed on the image. If the image is a fractal and self-similar, the D is independent of s

$$\int_{\ln(N1)}^{\ln(N2)} d\ln N = -\int_{\ln(s1)}^{\ln(s2)} D(s)\, d\ln(s)\ .$$

So that for a real fractal

$$N2 = N1\left(\frac{s2}{s1}\right)^{-D},$$

where $N2$ is the number of boxes of side $s2$ and $N1$ is the number of side $s1$.

If the microstructure is not self-similar, then D varies with s. In that case, we can treat the right hand side as a differential and integrate the small change with the trapezoidal rule to obtain

$$\ln(N2/N1) \approx -(D2+D1)[\ln(s2) - \ln(s1)]/2$$

and

$$N2 \approx N1\left(\frac{s2}{s1}\right)^{-\{D2+D1)/2}$$

where $D2$ and $D1$ are the D's at $s1$ and $s2$. Note that this is only true if $s1$ and $s2$ are close together and D changes slowly over that range.

The number of boxes we would predict to find at $s2$ if the system remained self-similar from $s1$ on is

$$N2_{SS} = N1\left(\frac{s2}{s1}\right)^{-D1}.$$

Microstructures are not fractals and are not expected to be self-similar. As the box size decreases, the rate of "all white box" generation will increase faster than the self-similar case. That loss can be equated to an areal change which is the largest for the box sizes closest to important spacing in the image.

The area reductions between $s1$ and $s2$ are

$$A = (N2_{SS} - N_2)s2^2.$$

Writing $s2 = s1+\Delta s$ and using $(1+\Delta s/s1)^{-D} \approx 1-D\Delta s/s1$ for small Δs, after some algebra one finds

$$\Delta A = (1/2)\ N1\ (\Delta s/s1)\ (D2 - D1)\ s2^2.$$

Since $s1 \approx s2$ we can drop the subscripts, and replace $N1$ by $N(s)$. By multiplying by $\Delta s/\Delta s$ we can treat $(D2-D1)/\Delta s \approx dD/ds$, and rewrite,

$$\Delta A(s) = s\, N(s)\, \Delta s^2\, (dD/ds)/2.$$

This is a distribution that can be normalized by dividing by

$$\int \Delta A(s) ds/\Delta s.$$

The number of boxes is found by dividing $\Delta A(s)$ by s^2,

$$\Delta N(s) = s^{-1}\, N(s)\, \Delta s^2\, (dD/ds)/2.$$

For image analysis, Δs is a constant, and is equal to the scaled width of a pixel. This expression gives a relationship between the area lost at important spacings in the spacing distribution, and the rate of change of the fractal dimension. For perfectly self-similar images, $\Delta A(s) = 0$ and $\Delta N(s) = 0$.

$\Delta A(s)$ and $\Delta N(s)$ might be related to a grain size distribution through modeling assumptions. However, that is difficult to do. The important point to be taken from this analysis is that the size of the activity is proportional to dD/ds. The peaks in the derivative are useful for identifying feature sizes of activity and verifying intuition about important grain size distributions in a microstructure.

2. Quantification of a Variation of the Secant Method

The secant method is a fast manual method in which a line of length S is drawn over a microstructure and the number of intersections is counted. Many secants are drawn with the number of intersections counted then averaged. It is easy to show that the average grain size returned by this method is $D_{sec} = S\langle 1/n\rangle_{ave}$; averaging S/n on each secant, the average grain size per secant. Also, $D'_{sec} = S/n_{ave}$; averaging n/S on each secant then inverting the average.

The latter can be very easily shown to be much quieter and accurate than the former.

A variation on the secant method is to record the intersection length for every intersection on every secant and average the intersection length values. When this is done, the average grain size determined by the variation of the method is

$$D_{int} = \Sigma\, l/N = TS/\Sigma\, n = S/(1/T)\Sigma\, n = S/n_{ave} = D'_{sec}.$$

where l is an intersection length, N is the total number of intersections, n is the number of intersections on a secant, and T is the total number of secants.

More information is available in the method that produced D_{int}. Suppose we make a histogram of the number of intersections that fall between l and $l+\Delta l$, using parallel secant lines that "scan" in a direction perpendicular to the lines, with the spacing between secants Δl. Now consider an image of a microstructure, and let Δl be the width of a single pixel. The length distribution would be the sum over all the *individual* grains of the number of times the spacing l occurred in each grain,

$$f(l,O) = \sum_G \eta_G(l,O).$$

The O designates the orientation to which the secant lines are perpendicular. G designates a grain.

This is a very simple expression. In order to relate it to a grain size distribution some assumptions about the make-up of the microstructure need to be made. Let us assume the following:

1. There is a number distribution of grain sizes in the microstructure, $n(g)$, where g is a grain size.
2. The grains have the same shape.
3. There is a function that tells us the number of times a length l occurs in a grain of size g. $q(l/g,O) = q(\beta,O)$, where the length parameter $\beta = l/g$.
4. The secant will move parallel to the largest length in the grains.

As an example, suppose there was a microstructure that was made up of all square shaped "grains" of different sizes filling space, and the secant line moves parallel to the diagonals. In that case, *q(unity,diag)* = 1 and *q(all others,diag)*=2. In grain of regular shape one would expect to find in a real microstructure the rate of change of q with respect to β is expected to be small. By assumption #4, we are defining the grain size to be the largest length in the grains. In the limit if circular grains, the secant lines will always be parallel to the length that defines the grain size. The latter also implies that $q(l/g) = 0$ for $g < 1$.

In reviewing these assumptions, it should be remembered that a large body of work exists on the characterization of grain size distributions in metals, where it is assumed that all grains are either circular or square, without considering the implications for the space-filling requirements.

The sum can now be taken over the grain sizes instead of individual grains, and written as

$$f(l,O) = \sum_{g\geq l}^{\infty} q(l/g,O)n(g) \cong \int_{l}^{\infty} q(l/g,O)n(g)\frac{1}{\Delta g}dg\,, \qquad (1)$$

where the Δg comes from passing the sum to an integral. The limits of the integration (or range of the sum) come from $g(l/g) = 0$ for $g < l$, since there can be no lengths in a grain that are greater than the grain size (by assumption #4). Equation 1 tells us that $f(l)$ is a *cumulative distribution*, most notably from the integral form.

To arrive at a relationship between $f(l)$ and $n(g)$ that might be extracted directly from data, consider from the summation that

$$f(l) - f(l+\Delta l) = \sum_{g\geq l}^{\infty} q(l/g)n(g) - \sum_{g\geq l+\Delta l}^{\infty} q(l+\Delta l/g)n(g).$$

The right hand side equals

$$q(\tfrac{l}{l})n(l) + q(\tfrac{l}{l+\Delta l})n(l+\Delta l) + q(\tfrac{l}{l+2\Delta l})n(l+2\Delta l) + \ldots - q(\tfrac{l+\Delta l}{l+\Delta l})n(l+\Delta l) + q(\tfrac{l+\Delta l}{l+2\Delta l})n(l+2\Delta l) + \ldots .$$

If q is constant or changes slowly such that

$$|\, q(\tfrac{l+\Delta l}{l+p\Delta l}) - q(\tfrac{l}{l+p\Delta l})\,| \,/\, q(\tfrac{l}{l+p\Delta l}) << |\, n(l+p\Delta l) - n(l+(p-1)\Delta l)\,| \,/\, n(l+p\Delta l)\,,$$

then terms containing $n(l+p\Delta l)$ are equal and only the very first term in the series remains in the difference, so that

$$n(l) \cong -\frac{\Delta g}{q(1)}\frac{\mathrm{d}f}{\mathrm{d}l} \quad \text{or} \quad n(l) \propto -\Delta g\frac{\mathrm{d}f}{\mathrm{d}l}. \qquad (2)$$

An alternative way of arriving at equation 2 is to rewrite equation 1 as the anti-derivative difference

$$f(l) = F(\infty) - F(l).$$

Differentiating both sides gives

$$\frac{\mathrm{d}f(l)}{\mathrm{d}l} = \frac{\mathrm{d}F(g=\infty)}{\mathrm{d}l} - \frac{\mathrm{d}F(g=l)}{\mathrm{d}l}.$$

The first term is zero, because $n(g) = 0$ for g significantly less than ∞, therefore, the anti-derivative at infinity must be equal to a constant. As for the second term, it must have the same functional form as the integrand of equation 1, resulting in

$$\frac{\mathrm{d}f(l)}{\mathrm{d}l} = -\frac{q(1)n(g)}{\Delta g},$$

which leads back to equation 2. Therefore, the assumptions about the slow rate of change of q are built into the conversion from sum to integral.

Consider that $F(g)$ is the anti-derivative of a distribution. $I = F(\infty) - F(0)$ is the total area beneath that distribution, in this case, the total number of intersections in the image. Unless the distribution is weighted very close to $g = 0$, $I \cong F(\infty)$.

Note that the O has been dropped, but the orientation dependence is implicit. The proportionality in Equation 2 is there since $q(l)$ is constant. Both derivations lead to the constant of proportionality $q(l)$, thus in grains of all the same shape, the only remaining influence from the shape function is the number of times the largest length g appears in the grains of size g.

The total area of the grains of size between l and $l+\Delta l$ is

$$\Delta A(l) \propto n(l) l^2. \tag{3}$$

In the above derivations, it is to be understood that the *l's* and *g's* and *s's* are equivalent as far as the histogram is concerned.

Grains are not square, nor do they have the same shape, so there is much uncertainty surrounding the entity $q(l/g)$. Given the wealth of work in which microstructures have been treated as though all the grains are squares or circles and the common equating of average secant intercept length to average grain size, we argue that $q(l/g) = constant$ will put this method on similar footing with more standard methods. Using $q=2$ seems reasonable for circles or diamond shaped grains.

It should be remembered that $f(l,O)$ is actually convolution of number of grains of size l and grain shape.

3. Application to a complicated microstructure

The assumptions made above are never going to be strictly true, but if they are good enough, then they would provide functional forms that would be useful for fitting data to real microstructures, and that is the most important test.

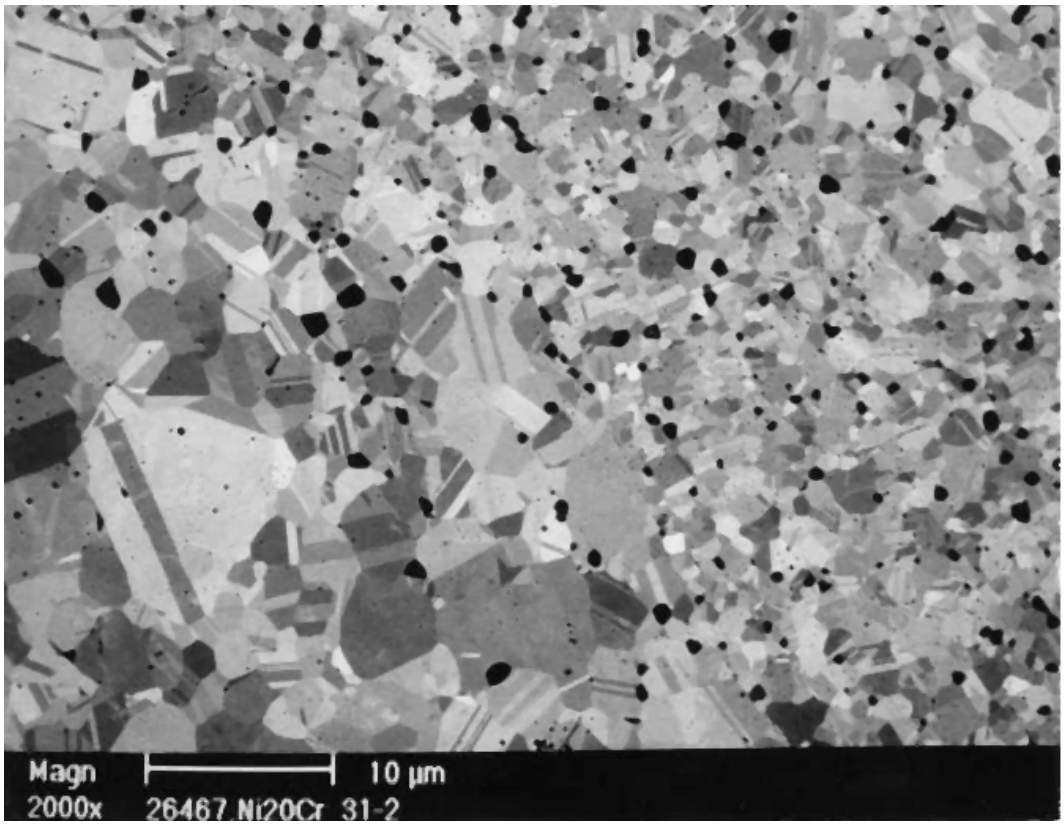
An example will be shown for a microstructure that is very complex. The figure below shows a microstructure that has either grain size gradients and/or overlapping grain size distributions. To make matters more complicated, the image does not show the full microstructure, which enhances gradients in the data.

Our image is of a specimen of cryomilled $Ni_{20}Cr$. It is smoothed in Scion Image, and converted to an edge image in the same program. To generate $D(l)$ and dD/dl it is analyzed in HarFA.

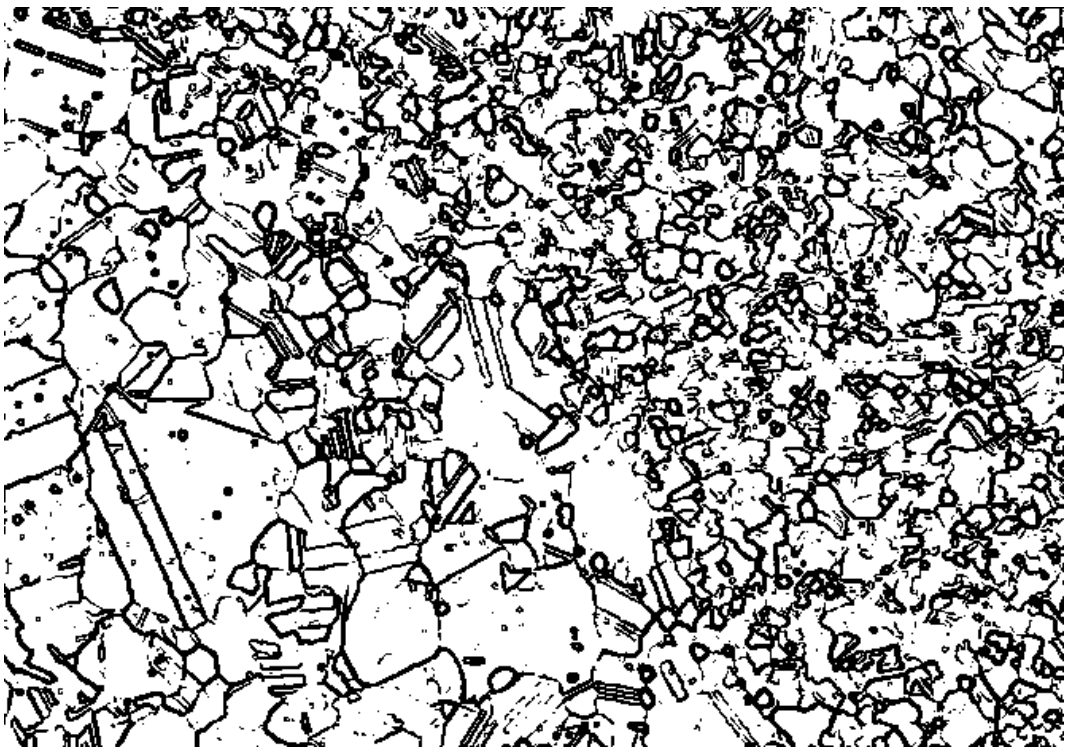
Using the intersection analyzer code called DA written at Rockwell, a histogram of 23,000 intersection lengths is created, $f(l)$. The data is then differentiated as per *Eqn. 1*.

Peaks are observed in dD/dl *vs.* $\sqrt{2}\,l$ and also df/dl *vs. 1*. These peak positions and widths are then combined to fit gaussian forms for *n(g)* that are integrated in *Eqn. 2* in order to fit $f(l)$. The gaussians are then differentiated, and the fit is compared to the df/dl data. As will be seen, the fits are reasonable. Fitting of the gaussians is done on $f(l)$ since differentiating produces noise.

Two additional ideas are incorporated. First, in the peak identification from dD/dl, the *l's* of the peaks are multiplied by $\sqrt{2}$ for the centers of the gaussians. This is because we believe the area is lost due to shrinking of the box *diagnols* below the spacing between grain boundaries. This correction does not have to be applied to the intersection spacings. Second, in Eqns. 1–3, we assume that $q(l/g) = 2$ for all l/g since it will be equal to two for the overwhelming majority of *l's* for space filling grains in the simple case where their shape is square.



Original Image



After Conversion to an Edge Image

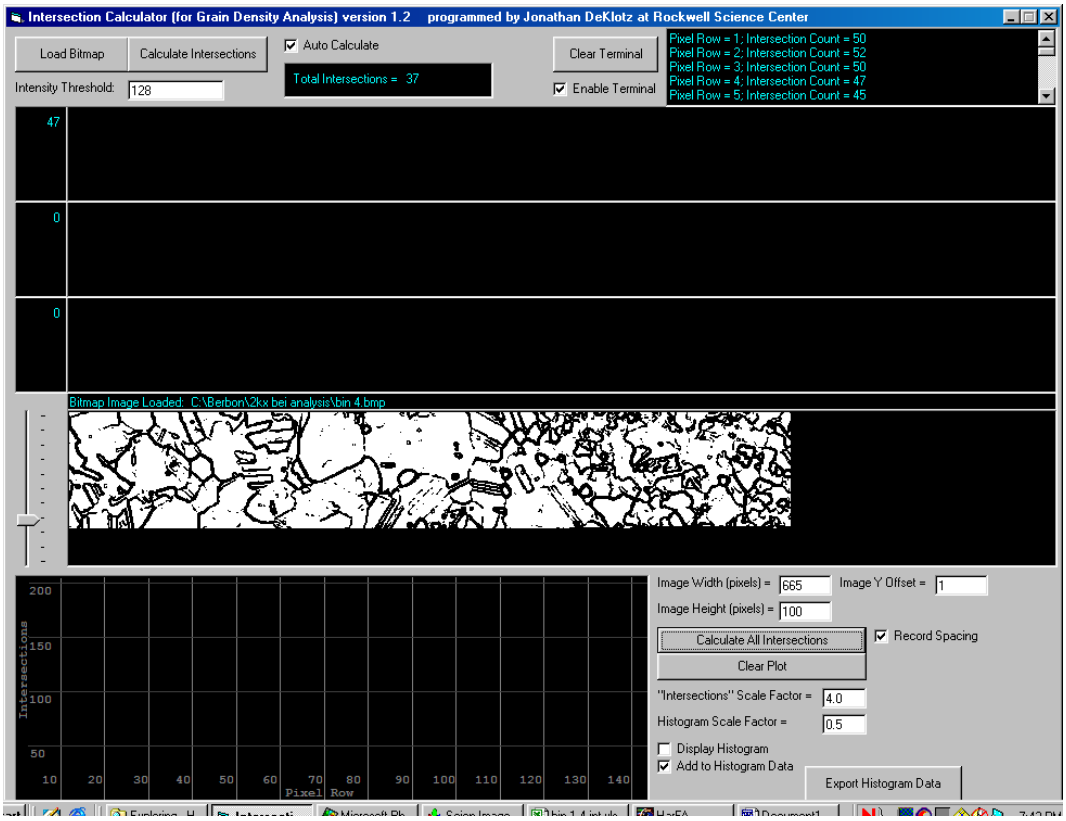


Figure 1 *Analyzing the image in the intersection analyzer to generate f(l).*

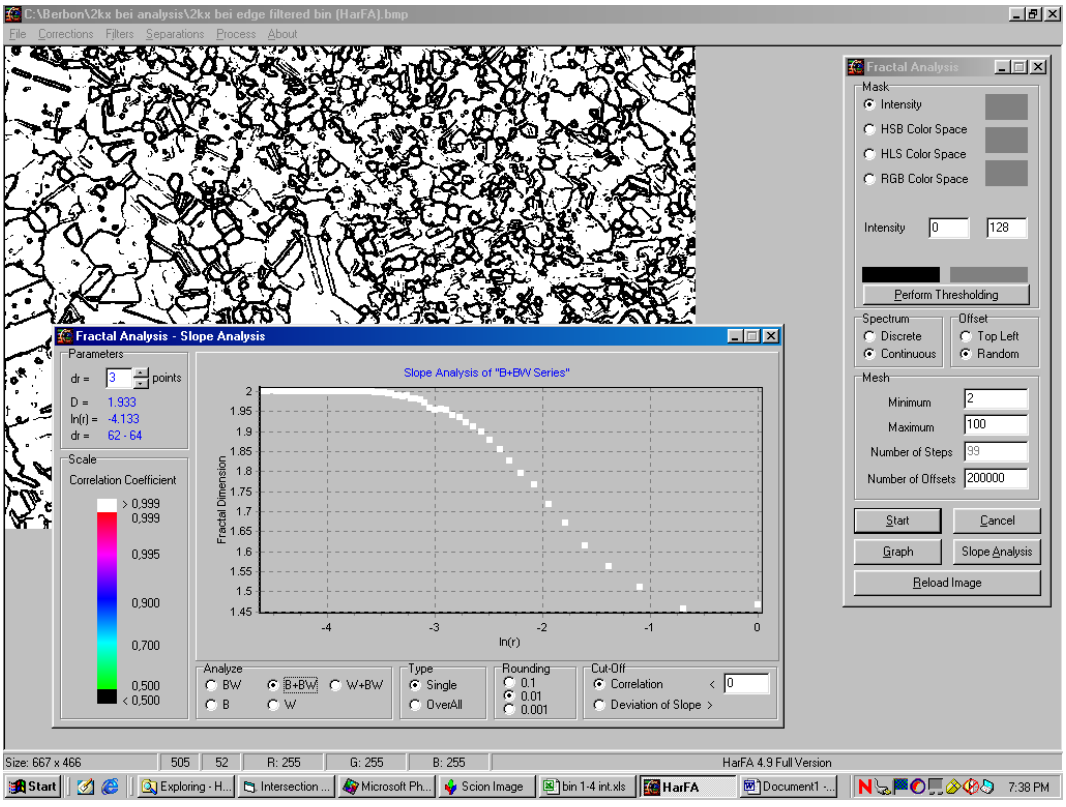


Figure 2 *Analyzing the image in HarFA to extract D(s) and* d*D*/d*s.*

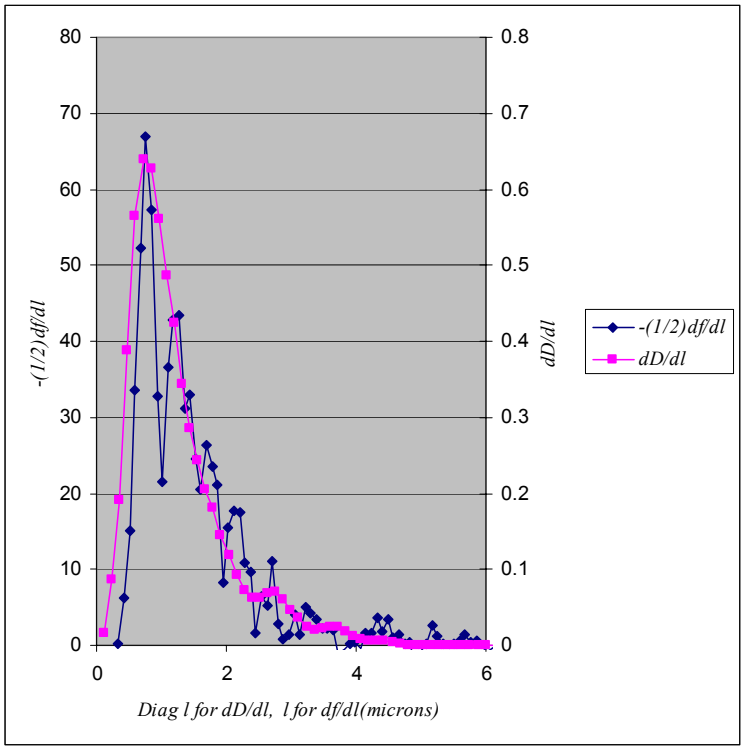


Figure 3 *Comparison of* d*D*/d*l and* d*f*/d*l showing the qualitative agreement. In both, the peaks at 0.76 microns and 2.76 microns match. The df/dl suggests activity at 1.27 microns as well. Those three, and no others, were used to fit gaussians to f(l) using Eqn. 2. Recall from Eqn. 1 that the grain size distribution n(g) = –*Δ*g/q(1) ×* d*f*/d*l.*

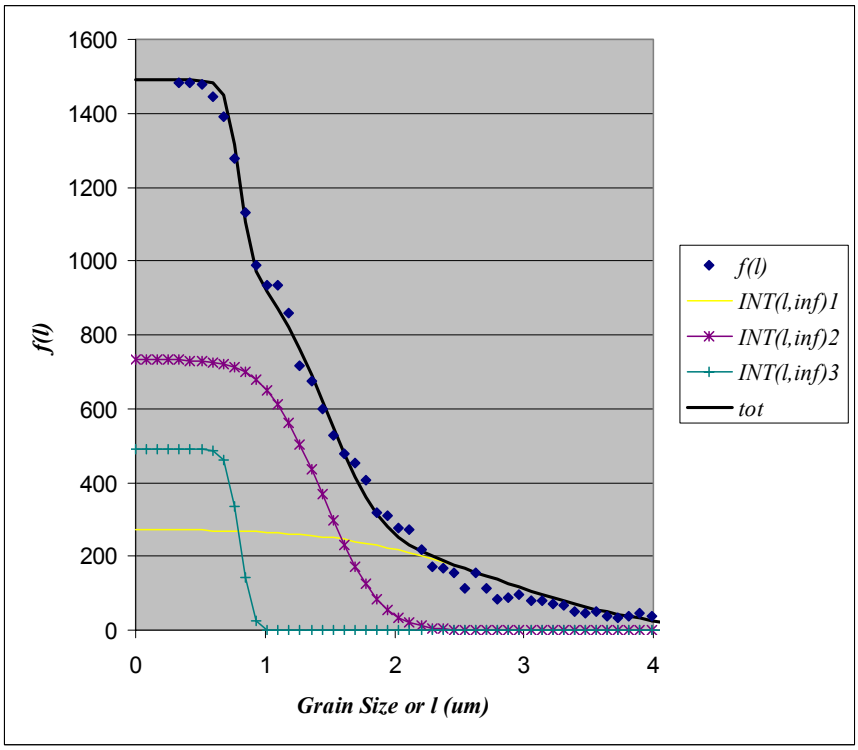


Figure 4 *Fit #1 to the data using Equation 2 and gaussians with peaks from the aforementioned dD/dl and* d*f*/d*l plots.*

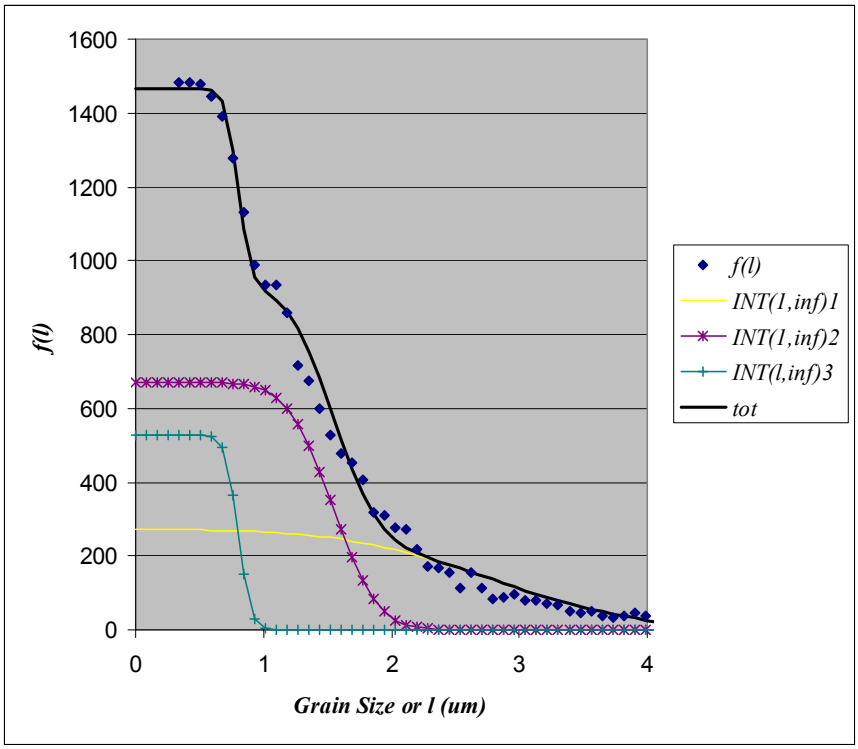


Figure 5 *Fit #2 to the data using Equation 2 and gaussians with peaks from the aforementioned* d*D*/d*l and* d*f*/d*l plots.*

Table 1 *The two sets of gaussians used on the fits.*

Gaussians	*1-#1*	*2-#1*	*3-#1*	*1-#2*	*2-#2*	*3-#2*
$2N_o$	10	70	195	10	80	210
l_o *(um)*	2.756	1.4	.76	2.756	1.5	.76
σ*(um)*	1.3	.5	.12	1.3	.4	.12

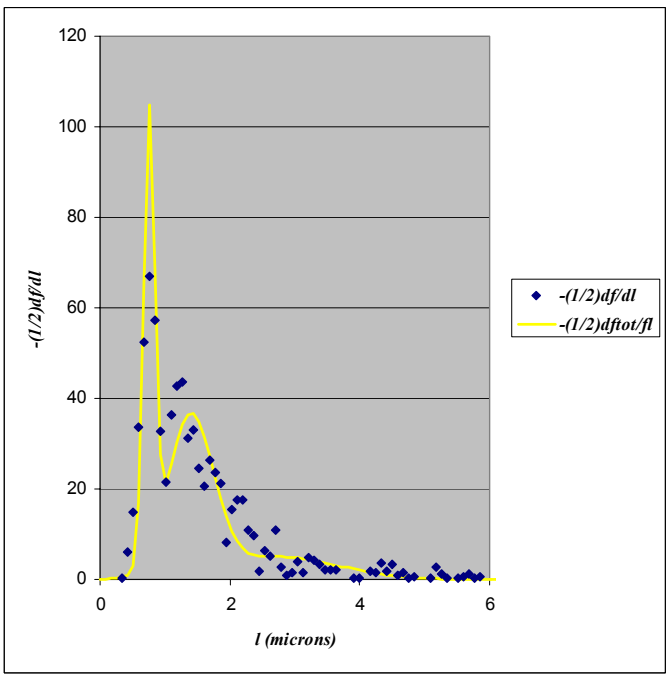


Figure 6 *The yellow line is the derivative of the fit to f*(*l*) *from Eqn 2, gaussian set #1.*

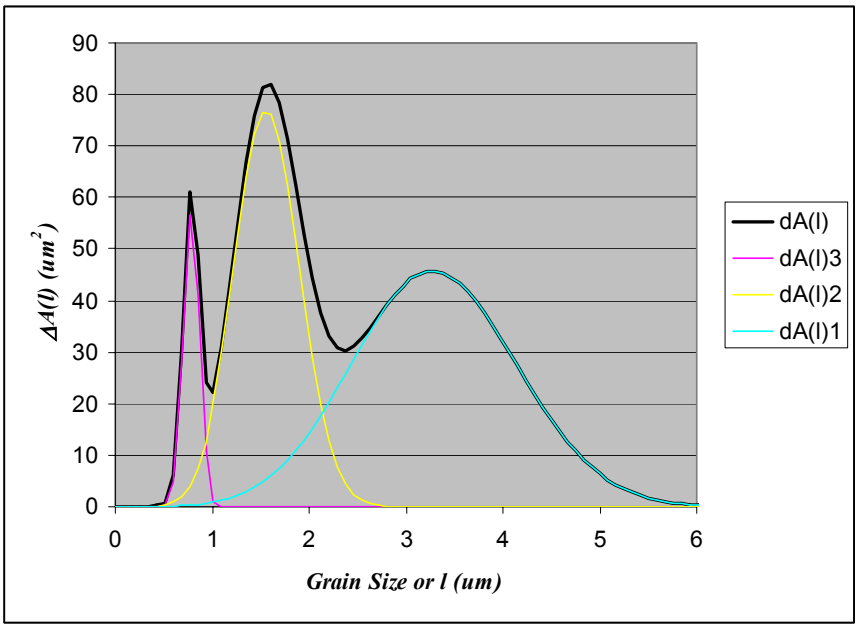


Figure 7 *The gaussians are multiplied by l^2 as per Eqn. 3 to get the areal distribution.*

Table 2 *Relative Areas of Grains in Distribution.*

	gauss#1	*gauss #2*	*gauss #3*
% Area	55.87	37.15	6.96
l_o*(um)*	2.756	1.4	0.76

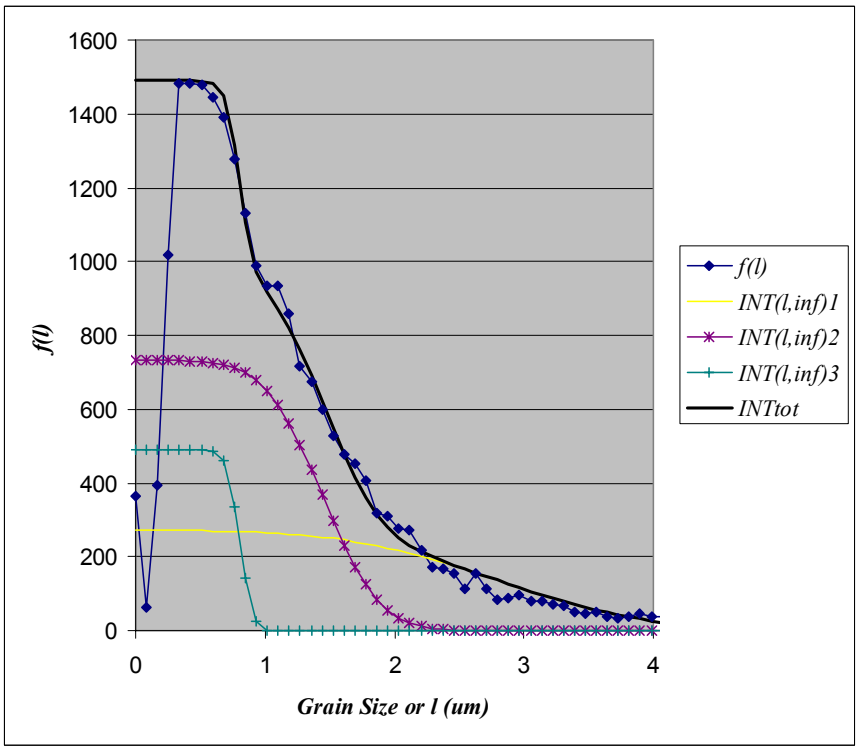


Figure 8 *This chart is a reminder that f(l,O) has grain shape dependence. Note that in the context of Eqn. 1, q(l/g,O)→ 0 for l < 0.25 microns.*

4. Discussion.

We are able to relate the fractal dimension derivative to length spectra from a variation on the secant method. The assumptions to relate the information to grain size distributions (Eqn. 1) are in need of comment, and though they are somewhat artificial, they are very similar to the assumptions that have been used to deal with grain shape in a large body of work on metals. The transformations on *f(l)* are performed to convert it into a representation of a grain size distribution, but it should be understood there are inherent errors. Good fitting to data *f(l)* and *df/dl* is possible from observations on the combined methods.

Consider the following perspective: it is often the case that the only information reported regarding the microstructure of a material is average grain size, sometimes with no mention of how it was determined. The figure actually reported may be the average of gradients or multiple distributions, and the omission of distribution information means that there is a gap in the literature relating material properties to size distributions (note the use of the words *size distributions* in general).

Also, note that emphasis is being put on fitting the *f(l)* with gaussians, with clues about where the gaussians are placed coming from the derivatives of *f(l)* and *D(s)*. This is because there is a lot of existing work on normal microstructures in which the distributions of secant intersection lengths and the average lengths in those studies are referred to as grain size distribution and average grain size.

Although the information generated by the methods in this paper may not be directly relatable to the usual definition of a grain size distribution, what is certain is that as the length scales of interfaces in materials fall through the nanoscale regime, all the intersection lengths in images will fall as well, along with average grain size. The distributions and fitting functions generated in this method offer additional means for standardizing reporting on the structure of polycrystalline materials. The method is fast and can be automated. The distributions derived can be just as easily correlated to physical properties of materials as average grain size.

The two methods under consideration do not show all of the same peaks. The d*D*/d*s* does not have the peak at 1.4 microns, but the d*f*/d*l* does. It is interesting to envision what the specific cases are that could describe the situation when there are fewer intersection lengths *l* counted in the image, yet there can be large amounts of all white box generation of side *l*. The case of harmonics is pictured below, in which boxes of size $s_o/2^m$ are shown for $m = 0$ and $m = 1$. For $s_o/2$ there are no lines of length $s_o/2$ directly associated with the white box generation, as there are for s_o.

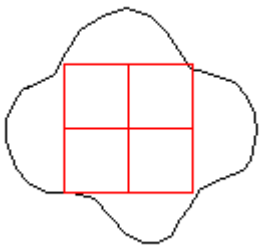


Figure 9 *Haromincs* s_o *(the large box) and* $s_o/2$ *(the quarters).*

The latter is not the case in our image, since the positions of the peaks of the fractal dimension do not follow a harmonic trend, $s = X_o/2^m$.

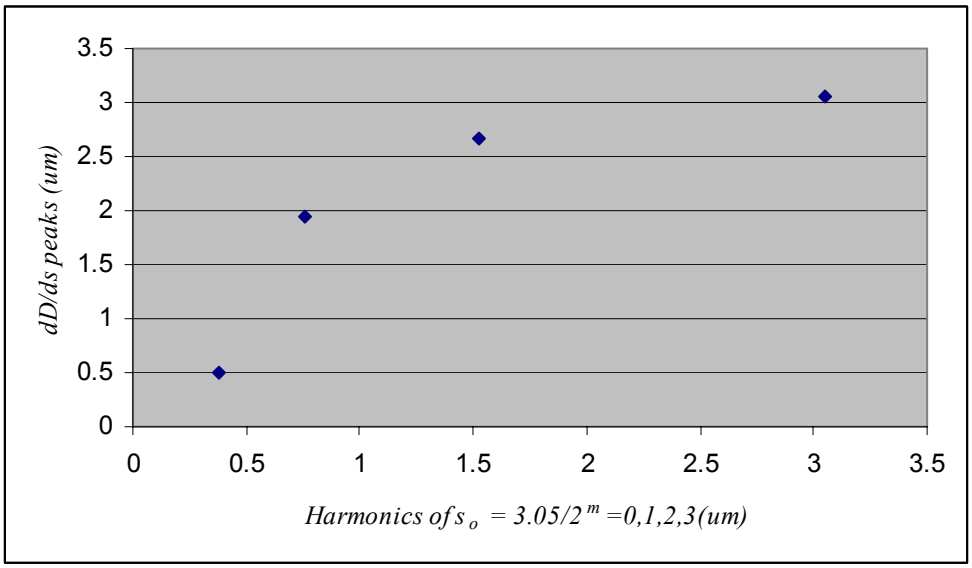


Figure 10 *No harmonic trend is seen for any value of X_o or progression of m, that is, a straight line of a slope of unity is not possible.*

5. Conclusions.

The lineal analysis produces *f*(*l*) which is a cumulative size distribution. The fractal analysis produces *D*(*s*). The positions of peaks in d*f*/d*l*, and d*D*/d*s* corresponding box diagonals give clues about where to place gaussians or other distributions shapes. Using the methods together is necessary, as the peaks in both methods do not always match.