Spectral analysis of randomly distributed scatterers for ultrasonic grain size estimation

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Since the average grain size is an important parameter in material characterization, the non-destructive evaluation of the microstructure in polycrystalline materials using ultrasonic backscattered echoes has significant practical implications. However, the complexity of the ultrasonic backscattered signal, which consists of interfering multiple echoes with random positions and amplitudes, makes accurate grain size evaluation difficult with conventional signal processing techniques. This Paper introduces an alternative approach which examines the spectrum of an ensemble of randomly distributed scatterers with known distribution to establish a relationship between the spectral and temporal statistical properties of the scatterers. Theoretical derivations based on a one-dimensional point scattered model show that the average grain size can be extracted from the power spectrum of the backscattered echoes. Using a non-linear least-squares technique, the theoretical grain power spectrum is curve-fitted to the sample grain power spectrum to estimate the mean and standard deviation of the grain size. Computer simulations based on this technique show that the average grain size can be extracted from the power spectrum of the backscattered echoes, indicating the potential feasibility of this technique for material characterization.

Keywords: material characterization; spectral analysis; random scatterer model; ultrasonic grain size estimation

Ultrasonic grain size estimation in polycrystalline materials using backscattered grain boundary echoes has significant practical implications in determining the quality and structural integrity of materials. The average grain size can be used to determine certain material characteristics which are relevant to non-destructive evaluation of materials. The most reliable grain size estimation is obtained by micrographic examination of samples, which is both destructive and time consuming since it involves polishing, etching and microscopically examining samples taken from the material[1]. Therefore, ultrasonic grain size estimation techniques have become a topic of interest in recent years and different techniques have been used with some success.

The ultrasonic wave travelling through solids is subject to scattering and mode conversion as the wave advances through the material and encounters the grain boundaries. Therefore, the received ultrasonic signal is a non-explicit function of the average grain diameter, ultrasonic wavelength, inherent anisotropic character of the individual grains, and the random orientation of crystallites[2,3]. Therefore, it has been possible to estimate the average grain size using the received ultrasonic signal.

A number of early studies examined the correlation between attenuation and material characteristics based on the decay of the transmitted pulse amplitude with distance using the reflections from the back surface of a sample consisting of two parallel surfaces[4-7]. Typically, the grain size estimation is obtained by comparing the ultrasonic attenuation in a specimen of unknown grain size with specimens of known grain size, while maintaining uniform test conditions. Although the attenuation measurement techniques provide an integrated grain size estimate in a relatively simple fashion, they are limited by surface irregularities, coupling, etc.[8,9]. More recently an alternative approach using backscattered echoes from the grain boundaries has been utilized by Fay[10,11] to determine the attenuation of ultrasound in materials with respect to depth or frequency. Based on the principle that ultrasonic waves travelling in solids are subject to scattering and absorption losses, Fay was able to demonstrate that the attenuation of the backscattered echoes with depth is related to the average grain size of the specimen. Goebbels *et al.*[8,12-14] later refined Fay's technique to more accurately determine the amplitude of the backscattered echoes with respect to depth by utilizing various averaging techniques. However, this approach results in the loss of localized grain size information and is not suitable if the backscattered echoes do not exhibit sufficient attenuation. Other techniques have also been examined which utilize the backscattered ultrasonic signal for grain size evaluation[15-17].

In this Paper, a new approach to grain size estimation based on spectral analysis of randomly distributed scatterers (i.e. RF signal) are utilized[18]. A theoretical model is developed to analyse the backscattered echoes from

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randomly distributed reflectors. Analytical calculations based on the statistical grain size model show that a relationship exists between the average grain size and the power spectrum of the received echo signal. Using a non-linear least-squares technique, the theoretical (i.e. statistical) grain power spectrum is curve-fitted to the actual (i.e. sample) grain power spectrum. The resulting curve-fitting parameters are then used to determine the average grain size and the standard deviation.

Spectrum of randomly distributed scatterers

For a one-dimensional random point scatterer model shown in *Figure 1* the response of a sample consisting of N scatterers can be defined as

$$g(t) = \sum_{i=1}^{N} a_i \delta(t - \tau_i) \qquad (1)$$

where a_i and τ_i are assumed to be uncorrelated random variables corresponding to the amplitude and position of the scatterers, respectively. Since the system is band limited, the received scatterer signal is the convolution of the scatterer function $g(t)$ and the system impulse response $h(t)$

$$r(t) = g(t) \otimes h(t) \qquad (2)$$

In Equation (1), the time of flight τ_i, which is the time between the reference point and the ith scatterer may be expressed as

$$\tau_i = \sum_{k=1}^{i} s_k \qquad i = 1, 2, \ldots, N \qquad (3)$$

where s_k is the individual time for the transmitted wave to traverse only the kth scatterer (see *Figure 1*). Because τ_i is the summation of statistically independent terms s_1 to s_i, its probability density function (pdf) can be expressed as the convolution of i individual pdf functions

$$f_{T_i}(\tau_i) = f_{s_1}(s_1) \otimes f_{s_2}(s_2) \otimes \ldots \otimes f_{s_i}(s_i) \qquad (4)$$

From probability theory[19], the characteristic function $\phi(\omega)$ of a random variable is the complex conjugate of the Fourier transform from its pdf. Therefore, the characteristic function of s_k is

$$\phi_{s_k}(-\omega) = E\{\exp(-j\omega s_k)\} = F\{f_{s_k}(s_k)\} \qquad (5)$$

where $\omega = 2\pi f$. If we assume that the time increments between individual scatterers s_1 to s_i are independent and identically distributed (iid), the characteristic function of τ_i becomes[19]

$$\phi_{T_i}(-\omega) = E\{\exp(-j\omega s_1)\} E\{\exp(-j\omega s_2)\} \ldots E\{\exp(-j\omega s_i)\} = \phi_s^i(-\omega) \qquad (6)$$

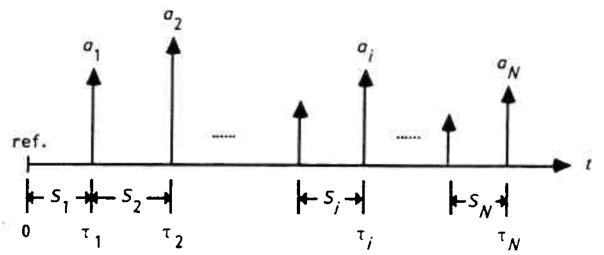

Figure 1 One-dimensional model for randomly distributed scatterers

The scatterer spectrum $G(\omega)$ can be obtained by taking the Fourier transform of Equation (1), as

$$G(\omega) = \sum_{i=1}^{N} F\{a_i \delta(t - \tau_i)\} = \sum_{i=1}^{N} a_i \exp(-j\omega\tau_i) \qquad (7)$$

Since a_i and s_i are assumed to be uncorrelated and individually iid, from Equations (6) and (7) the statistical scatterer spectrum $E\{G(\omega)\}$ becomes

$$E\{G(\omega)\} = \sum_{i=1}^{N} E\{a_i \exp(-j\omega\tau_i)\} = \mu_A \sum_{i=1}^{N} \phi_s^i(-\omega)$$
$$= \mu_A \frac{[1 - \phi_s^N(-\omega)]\phi_s(-\omega)}{1 - \phi_s(-\omega)} \qquad (8)$$

where μ_A is the mean of a_i and $\phi_s(\omega)$ is the characteristic function of s_k, the time of flight for each scatterer. Therefore, the statistical scatterer power spectrum can be obtained from Equation (8) as

$$|E\{G(\omega)\}|^2 = \mu_A^2 \frac{|1 - \phi_s^N(-\omega)|^2 |\phi_s(-\omega)|^2}{1 - [\phi_s(-\omega) + \phi_s^*(-\omega)] + |\phi_s(-\omega)|^2} \qquad (9)$$

where * denotes a complex conjugate. Therefore, for any scatterer distribution for which the characteristic function exists, the statistical scatter power spectrum can be obtained using Equation (9). To demonstrate this, two different scatterer pdfs are considered below:

1 if the scattered spacing s is assumed to be Gaussian distributed with mean μ and standard deviation σ, then its characteristic function becomes

$$\phi_s(\omega) = \exp(j\mu\omega - 0.5\sigma^2\omega^2) \qquad (10)$$

Hence, the statistical scatterer power spectrum $|E\{G(\omega)\}|^2$ becomes

$$|E\{G(\omega)\}|^2 = \mu_A^2 \frac{[1 - 2\exp(-0.5N\sigma^2\omega^2)\cos(N\mu\omega) + \exp(-N\sigma^2\omega^2)]\exp(-\sigma^2\omega^2)}{1 - 2\exp(-0.5\sigma^2\omega^2)\cos(\mu\omega) + \exp(-\sigma^2\omega^2)} \qquad (11)$$

2 if the scatterer spacing s is assumed to be uniformly distributed with mean μ and standard deviation σ, then the characteristic function becomes

$$\phi_s(\omega) = \mathrm{sinc}(\sqrt{3}\sigma\omega)\exp(j\mu\omega) \qquad (12)$$

Therefore, the statistical scatterer power spectrum becomes

$$|E\{G(\omega)\}|^2 = \mu_A^2 \frac{[1 - 2\,\mathrm{sinc}(\sqrt{3}N\sigma\omega)\cos(N\mu\omega) + \mathrm{sinc}^2(\sqrt{3}\sigma\omega)]\,\mathrm{sinc}^2(\sqrt{3}\sigma\omega)}{1 - 2\,\mathrm{sinc}(\sqrt{3}\sigma\omega)\cos(\mu\omega) + \mathrm{sinc}^2(\sqrt{3}\sigma\omega)} \qquad (13)$$

By examining Equations (11) and (13) for different μ and σ values, it can be shown that:

1 the statistical scatterer power spectrum is neither white nor monotone, but exhibits nearly periodic peaks;
2 the frequency spacing between these spectral peaks (Δf) and the average scatterer spacing (μ) have an inverse relationship;
3 as σ increases, the peaks of the statistical scatterer power spectrum will widen and the magnitude of the higher order harmonics will reduce more rapidly with frequency;

4 for mean-to-standard deviation ratio $\mu/\sigma < 4$, the statistical scatterer power spectrum peaks become relatively smooth making their detection more difficult;
5 in general, the shape of the statistical power spectrum will depend on the scatterer pdf even for fixed μ and σ values. However, the differences will diminish as μ/σ becomes large.

In conclusion, the theoretical results indicate that the statistical scatterer power spectrum is uniquely determined by the scatterer pdf and can be used for various signal processing and filter design applications (e.g. Wiener filter design). More importantly, the results indicate that it should be possible to estimate the statistical scatterer parameters using signal processing techniques. In the following section, the application of this technique for grain size estimation will be examined.

Grain size estimation based on scatterer model

The randomly distributed scatterer model described in the previous section can be used to represent grain boundaries if the following assumptions are satisfied[1]:

1 there is only elastic discontinuity at the grain boundaries (i.e. no discontinuity in density);
2 the energy due to multiple scattering is negligible (i.e. Rayleigh scattering is assumed since the ultrasonic wavelength is generally much larger than the average grain size);
3 the total scattering effect of grains may be approximated by an equivalent sphere;
4 the grain boundaries are randomly distributed in the specimen.

The relationship between grain size l_k and the corresponding ultrasonic round-trip time of flight s_k is given by

$$l_k = \frac{cs_k}{2} \qquad (14)$$

where c is the sound velocity in the sample and the factor of 2 results due to the round-trip time. If the grain size is iid and has Gaussian distribution with mean μ_l and standard deviation σ_l, the statistical grain power spectrum can be obtained from Equations (11) and (14) as

$$|E\{G(\omega)\}|^2 = \mu_A^2 \frac{\left[1-2\exp\left(-\frac{2N\sigma_l^2}{c^2}\omega^2\right)\cos\left(\frac{2N\mu_l}{c}\omega\right)+\exp\left(-\frac{4N\sigma_l^2}{c^2}\omega^2\right)\right]\exp\left(-\frac{4\sigma_l^2}{c^2}\omega^2\right)}{1-2\exp\left(-\frac{2\sigma_l^2}{c^2}\omega^2\right)\cos\left(\frac{2\mu_l}{c}\omega\right)+\exp\left(-\frac{4\sigma_l^2}{c^2}\omega^2\right)} \qquad (15)$$

It is clear that the statistical grain power spectrum $|E\{G(\omega)\}|^2$ is a function of frequency, average grain size (μ_l), standard deviation (σ_l) and the number of grains (N). The statistical grain power spectrum defined by Equation (15) is plotted in *Figure 2* for different values of μ_l and σ_l. Note that the spectral peaks centred at DC have been excluded from the plots since they contain no information related to the average grain size and have large amplitudes which prevent the subsequent peaks from being observed on the same scale. It is clear from *Figure 2* that there exists an inverse relationship between the peak locations and the average grain size. In addition it can be shown that the width of the spectral peaks increases as σ_l becomes larger.

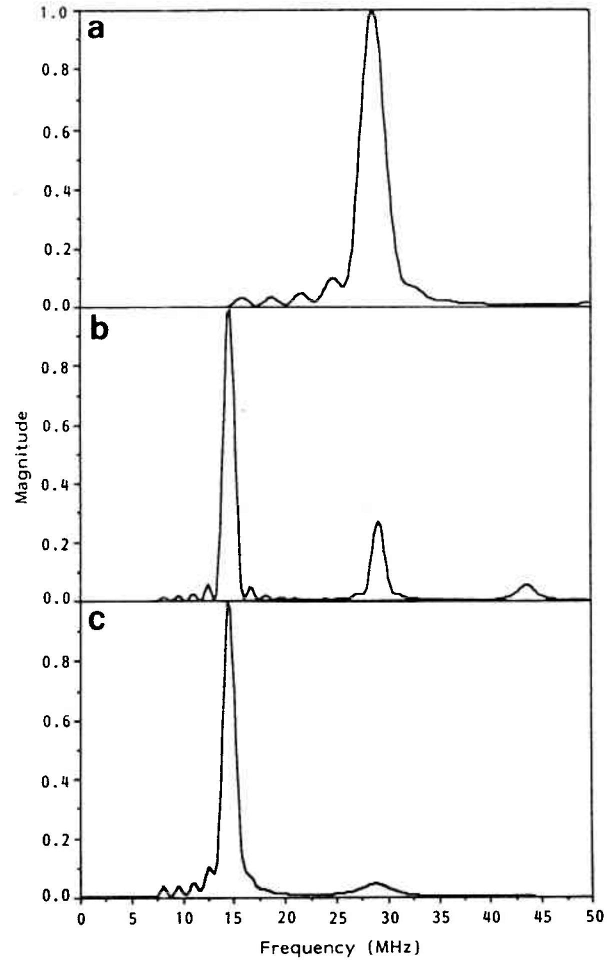

Figure 2 Statistical grain power spectrum. (a) $\mu_l = 100$ μm, $\sigma_l = 10$ μm; (b) $\mu_l = 200$ μm, $\sigma_l = 10$ μm; (c) $\mu_l = 200$ μm, $\sigma_l = 20$ μm

Note that for infinitesimal values of σ_l Equation (15) becomes

$$\lim_{\sigma_l \to 0} |E\{G(\omega)\}|^2 = \mu_A^2 \frac{1-\cos\left(\frac{2N\mu_l}{c}\omega\right)}{1-\cos\left(\frac{2\mu_l}{c}\omega\right)} = \mu_A^2 \left[\frac{\sin\left(\frac{N\mu_l}{c}\omega\right)}{\sin\left(\frac{\mu_l}{c}\omega\right)}\right]^2 \qquad (16)$$

Equation (16) is a special case of Equation (15) and results in periodic pulses with frequency spacing Δf, which is related to the average grain size μ_l as

$$\Delta f = \frac{c}{2\mu_l} \qquad (17)$$

Therefore, when σ_l is small compared with μ_l, this relationship can be used to estimate the average grain spacing. Note that Δf will essentially remain fixed for non-zero values of σ_l. However, as σ_l increases, the peaks of the statistical grain power spectrum will widen and the magnitude of the higher order harmonics will reduce more rapidly with frequency, possibly making grain size estimation difficult. In general, if $\mu_l/\sigma_l \geq 4$, then the first peak to the grain power spectrum can be detected conveniently and used to estimate the average grain size. Furthermore, the standard deviation of the grain size may be estimated from the bandwidth of the first peak. Finally, it can be shown that for large N and non-zero σ_l Equation (15) simplifies to

$$|E\{G(\omega)\}|^2 = \mu_A^2 \frac{\exp\left(-\frac{4\sigma_l^2}{c^2}\omega^2\right)}{1 - 2\exp\left(-\frac{2\sigma_l^2}{c^2}\omega^2\right)\cos\left(\frac{2\mu_l}{c}\omega\right) + \exp\left(-\frac{4\sigma_l^2}{c^2}\omega^2\right)} \tag{18}$$

Based on the above results, the grain parameters μ_l and σ_l can be determined by comparing the statistical grain power spectrum $|E\{G(\omega)\}|^2$ in Equation (18) with the sample grain power spectrum $|G(\omega)|^2$ obtained from experimental specimens or by simulation. The estimation error is defined as

$$\varepsilon^2 = \int_{2\pi(f_1-\rho/2)}^{2\pi(f_1+\rho/2)} \| G(\omega)|^2 - \lambda |E\{G(\omega)\}|^2|^2 \, d\omega \tag{19}$$

where $f_1 = \Delta f$ and ρ are the centre frequency and bandwidth of the first spectral peak, respectively, and λ is the normalization constant. Therefore, if N (the total number of grains) is sufficiently large, Equations (18) and (19) can be used to estimate the grain statistics. The average grain size μ_l, standard deviation σ_l and normalization constant λ can be obtained by minimizing ε^2 with respect to μ_l, σ_l^2 and λ. This is accomplished by setting the corresponding derivatives equal to zero and solving the resulting equations simultaneously

$$\frac{\partial \varepsilon^2}{\partial \mu_l} = 0 \qquad \frac{\partial \varepsilon^2}{\partial \sigma_l^2} = 0 \qquad \frac{\partial \varepsilon^2}{\partial \lambda} = 0 \tag{20}$$

In the following section the above technique will be examined using computer simulations.

Simulation results

The estimation process described earlier is examined here using simulated data. The system impulse response $h(t)$ is modelled as an exponentially decaying cosine wave

$$h(t) = \exp(-B|t|)\cos(2\pi f_0 t) \tag{21}$$

where $f_0 = 15.0$ MHz is the centre frequency and $B = 3.3$ MHz is the 6 dB bandwidth. Therefore, the received (i.e. backscattered) grain signal can be generated using Equations (1), (2) and (21)

$$r(t) = \sum_{i=1}^{N} a_i \exp(-B|t-\tau_i|)\cos[(2\pi f_0(t-\tau_i)] \tag{22}$$

The time of flight τ_i can be obtained from the following equation

$$\tau_i = \frac{2}{c}\sum_{k=1}^{i} l_k \tag{23}$$

where c is the sound velocity in the medium and l_k is the random grain size, which is Gaussian with mean $\mu_l = 150$ μm and standard deviation $\sigma_l = 20$ μm. The simulation also assumes that a_i is Gaussian with mean 0.5 and standard deviation 1.0. The following simulated signals are generated based on a sampling frequency $f_s = 100$ MHz (i.e. sampling period of 10^{-8} s) and sound velocity of $c = 5800$ m s^{-1}. The system impulse response is shown in *Figure 3* and the received grain signal in *Figure 4*.

The sample grain power spectrum $|G(\omega)|^2$ is required to estimate the grain size parameters and can be obtained from $r(t)$ by deconvolution

$$|G(\omega)|^2 = \frac{|R(\omega)|^2}{|H(\omega)|^2} \tag{24}$$

where $R(\omega)$ is the received grain spectrum and $H(\omega)$ is the system transfer function. The spectra terms in Equation (24): $|R(\omega)|^2$, $|H(\omega)|^2$ and the deconvolved power spectrum $|G(\omega)|^2$ are shown in *Figures 5–7*, respectively. As expected from theoretical derivations, there exists a frequency peak in the deconvolved sample grain power spectrum shown in *Figure 7*, which should correspond to the average grain size. The results are analysed further in the following section to ascertain this observation.

Because the statistical grain power spectrum is a non-linear function, more than one local minimum may exist. Therefore, the initial value for the estimation parameters should be selected properly. It can be shown that the initial value selected for μ_l is much more critical to the estimation process than σ_l. Therefore, if the first peak frequency f_1 can be identified from the deconvolved sample grain power spectrum (see *Figure 7*), the initial

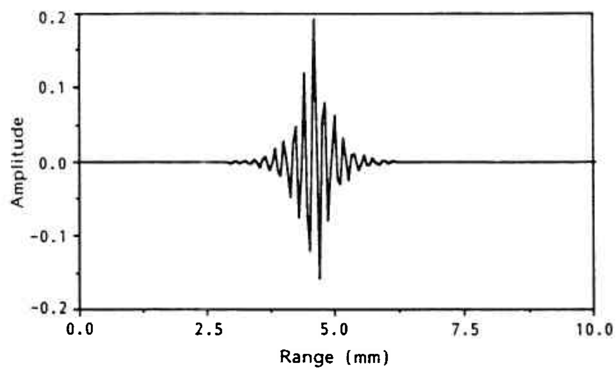

Figure 3 System impulse response $h(t)$

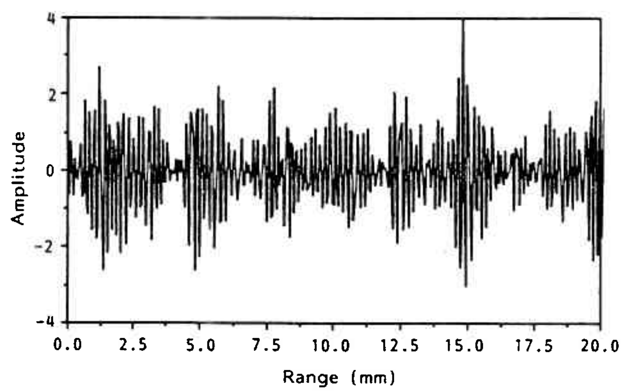

Figure 4 Simulated grain signal $r(t)$

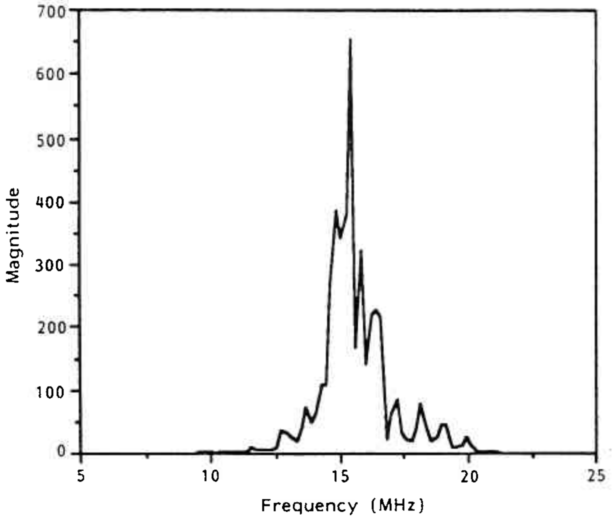

Figure 5 Received grain power spectrum $|R(\omega)|^2$

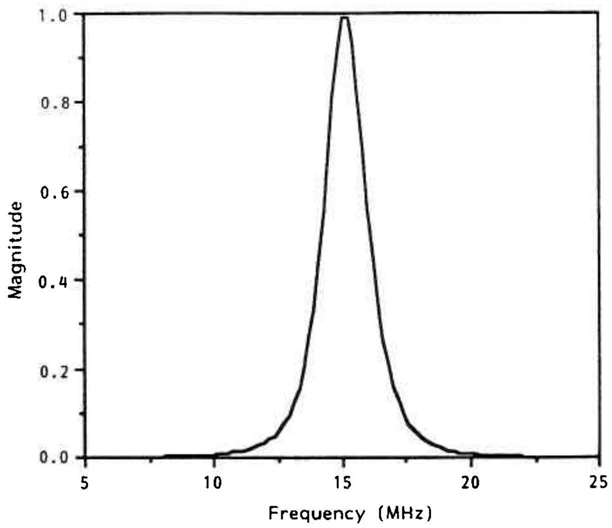

Figure 6 System power spectrum $|H(\omega)|^2$

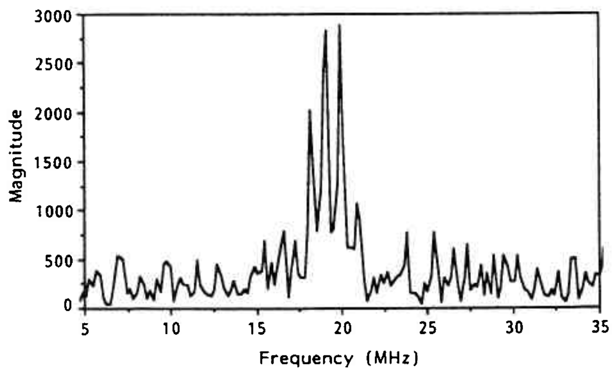

Figure 7 Sample grain power spectrum $|G(\omega)|^2$

estimate for the mean grain size μ_l can be determined using

$$\mu_l = \frac{c}{2f_1} \tag{25}$$

The selection of the initial value for the standard deviation σ_l is arbitrary, as long as it is smaller than the mean. The second task is the selection of the spectral region where the estimation is performed (i.e. curve fitting region). Since the sample grain power spectrum $|G(\omega)|^2$ converges to the statistical grain power spectrum $|E\{G(\omega)\}|^2$ within the neighbourhood of the first frequency peak f_1, the grain size parameter estimation is performed within this region. In general, this range may fall outside the 6 dB bandwidth of the system. Therefore, high signal-to-noise ratio (SNR) data must be used to obtain reliable grain size estimation. In practice this can be accomplished by time averaging the experimental data to remove any random system noise such as thermal receiver noise.

The process essentially curve fits the statistical grain power spectrum $|E\{G(\omega)\}|^2$ (see Equation (18)) to the simulated (or experimental) sample grain power spectrum $|G(\omega)|^2$ (see Equation (24)) by selecting the estimation parameters μ_l, σ_l and λ which minimize the error in Equation (19). Once the curve fitting range and the initial values for μ_l and σ_l are determined, the curve fitting is accomplished using a standard non-linear estimation software package. *Figure 8* shows the curve fitting plots in the frequency range $16 < f < 23$ MHz. The procedure results in the final estimation values shown in *Table 1*, which agree closely with the simulation parameters.

To further evaluate the performance of the grain size estimation technique, a group of simulations were performed. The simulated data were first analysed by fixing the standard deviation of grain size at $\sigma_l = 25$ μm, while the average grain size μ_l was changed from 100 to 300 μm. For each value of μ_l, five independent data sets were generated and processed by the above estimation technique. *Figure 9* shows the estimation results for each μ_l. Note that the estimation error for each data set is small, especially for large μ_l.

Next, the average grain size was fixed at $\mu_l = 150$ μm, while the standard deviation σ_l was changed from 5 to 25 μm. For each value of σ_l, five independent data sets were generated and processed to determine the corresponding estimation parameters, which are shown in *Figure 10*. As expected, the estimation becomes less

Table 1 Estimation results

	μ_l (μm)	σ_l (μm)
Actual data	150	19.7
Estimated data	149	21.6
Relative error (%)	0.67	9.6

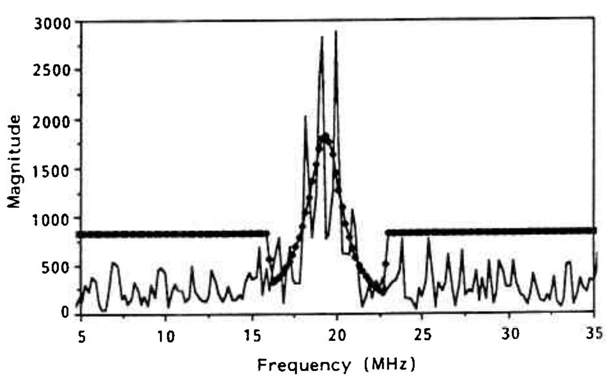

Figure 8 Spectral curve fitting result. ——, $|G(\omega)|^2$; —●—, $|E\{G(\omega)\}|^2$

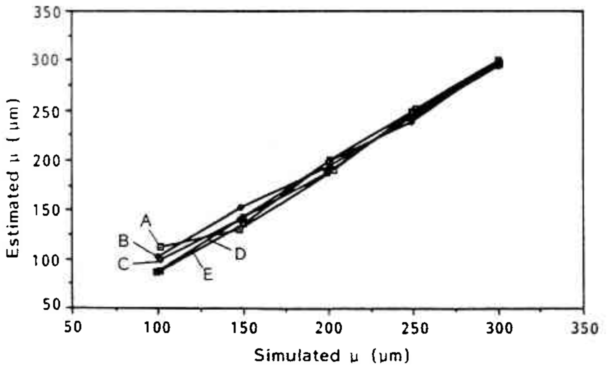

Figure 9 Estimation results for μ_l with fixed $\sigma_l = 25$ μm. A, est. 1; B, est. 2; C, est. 3; D, est. 4; E, est. 5

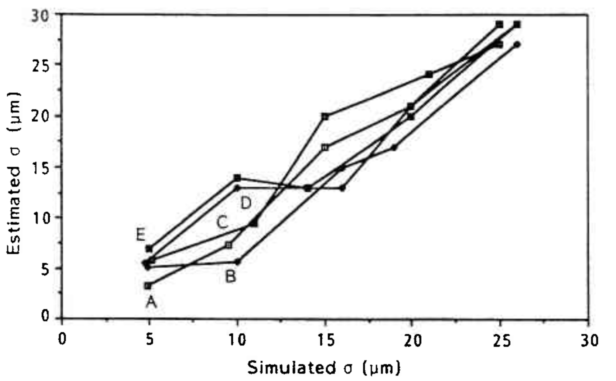

Figure 10 Estimation results for σ_l with fixed $\mu_l = 150$ μm. A, est. 1; B, est. 2; C, est. 3; D, est. 4; E, est. 5

accurate as the standard deviation increases, which is evident in *Figure 10*. Although the estimation error for σ_l is relatively large compared with the estimation of μ_l, it is still within an acceptable range.

Practical considerations and feasibility

As shown in the previous section, the statistical parameter estimation technique developed can successfully determine the mean and standard deviation of the grain size in one-dimensional computer simulations. Since the periodic spacing of the peaks in the statistical grain power spectrum was shown to be inversely proportional to the average grain size in Equation (17), the average grain size can be estimated either by using the first peak location in the spectrum or the frequency spacing between subsequent peaks. In general, it is preferable to base the estimate on the frequency of the first peak since it will exhibit the largest amplitude thus making it easier to locate. However, there are several factors and physical limitations which must be considered in practical applications. First, there are limitations imposed by the transducer and/or system bandwidth. Therefore, the grain sizes which can be estimated experimentally by the spectral technique must correspond to the frequencies within the transducer pass band. When the spectral peaks occur outside the transducer frequencies, the curve fitting technique will fail to detect them. Although improving the SNR by signal averaging and increasing the spectral range by deconvolution will help, it cannot overcome the basic system bandwidth limitations. To give a practical example, if the average grain size for a stainless steel sample is 100 μm, the first peak of the grain power spectrum can be calculated from Equation (25) as $f_1 = 29$ MHz, which is too high for most typical transducers to detect. Since it is not physically possible to use a single ultrasonic transducer with bandwidth large enough to permit the estimation of a wide range of practical grain sizes, the transducer should be selected to match the particular range of grain sizes expected in the samples being tested. In addition, to improve the algorithm performance (especially at the tail ends of the transducer pass band) it is essential that the experimental data have high signal-to-noise ratio, which can be achieved by time averaging during data acquisition.

Second, practical limitation is related to the statistical distribution of grains. As discussed earlier, when the standard deviation of the grain size (σ_l) increases relative to the mean grain size, it becomes more difficult to locate the first peak in the grain power spectrum. Therefore, this technique may not be practical for testing samples having small mean-to-standard deviation ratio μ_l/σ_l. However, this limitation is not inherent to the proposed algorithm but will adversely affect any parameter estimation technique.

Since the simulation results are highly encouraging, experimental testing is recommended using known test samples to evaluate the feasibility of the grain size estimation technique for practical applications. The experimental evaluation should focus on large grained specimens which can be tested using conventional transducers (i.e. 5–20 MHz centre frequencies). Initial tests should be performed using carefully selected test samples with known grain statistics. It is believed that the statistical grain size estimation technique described here can be improved by developing a more generalized grain model, which takes into account such factors as attenuation, anisotropy, multiple scattering, correlation between grain size and echo amplitudes, etc.

Conclusions

The technique presented here is a novel approach in grain size estimation. The concept is based on the spectral analysis of randomly distributed scatterers and utilizes a non-linear least-squares parameter estimation technique to determine the mean and standard deviation of the grain size. The technique has been tested extensively using computer simulations, which have shown that accurate grain size estimation can be achieved when the ratio between the average grain size and its standard deviation is approximately 4 or larger. Since the simulation results are encouraging and indicate the feasibility of this technique for practical applications, further study and experimental testing of the technique is recommended. In addition, it is believed that the one-dimensional grain model can be refined to improve the accuracy of grain size estimation by including the affects of attenuation, multiple scattering, etc. Finally, it is essential that wideband transducers are utilized in practical applications to ensure versatility and large dynamic range.

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