ABERRATION IN POLYCRYSTALLINE MATERIALS

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ABSTRACT. Many materials contain a random microstructure that can have an adverse effect on ultrasonic measurements (reducing signal strength, increasing noise and reducing accuracy) through scattering and aberration of the acoustic field. To account for those adverse effects we have developed a phase screen model alongside the stochastic wave equation. This two fold approach allow us to directly model the field for adaptive correction and to characterise material from the statistical properties of experimental measurements.

INTRODUCTION

Materials like aluminium and steel that consist of many crystallites or grains on their micro scale are called polycrystalline materials. The importance for their characterisation by means of obtaining the grain size distribution has been long recognised among the nondestructive testing community. Most studies dealing with microstructure evaluation are based on estimation of attenuation coefficient for ultrasonic waves propagated in polycrystalline materials. The attenuation coefficient is obtained by looking at the first moment of the acoustic field in the stochastic approach being backscattered a key role. Not only is the backscatter important in ultrasonic evaluation but also wavefront distortion or aberrations that an acoustic wave suffers as it propagates in the material. Aberrations are random functions that can be observed in a speckle pattern by imaging the ultrasonic field using a c-scan technique [1]. In this paper we present a statistical study of aberrations using a c-scan technique to obtain speckle pattern of acoustic field for surface acoustic waves. The interpretation of aberrations caused by the microstructure has been supported by simulating them using scalar stochastic and phase screen theory. Therefore, one of the purposes of this paper is to analyse approximate solutions to stochastic Helmholtz's equation that may represent aberrations of acoustic waves effectively in inhomogeneous random medium. All these approximations have been applied to different situations and most methods are reviewed elsewhere, [2, 3]. In particular we are interested in the parabolic approximation to Helmholtz's equation, which has been studied in [2, 3] and its relationship to phase screen approach, which is well known in optics [4]. In [5] and references therein the authors showed that aberrations in polycrystalline materials can be simulated using phase screen approach. The authors simulated microstructure using numerical techniques to simulate grain growth and to build grains boundaries. Taking into account grain growth, screens were designed accordingly to grain boundary geometry in a real material to randomly distort the phase velocity of an incident acoustic wave to a random media. Those ideas for simulating aberrations [5] will be used in this paper, however, screens will be designed by assuming some predefined statistical properties for the random function representing properties of the medium in the scalar description. These two points of

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view are interconnected and its connection is made by defining the screens as a function of the wave number, as noted in [6] and references therein.

The second order moment or coherence function is the key in understanding the relationship between aberrations and microstructure. The half-width of the coherence function is a measure of the size of the speckle pattern and it is believed to be a measure of grain size of the material on interrogation. The ensemble averaging of speckle patterns requires multiple measurements obtained by changing the detector and source position across the surface of the sample. In that way it was possible to measure the average coherence function for aluminium and compare this to theory to obtain information of grain size. The apparatus used to perform the c-scan at fundamental frequency of 82 MHz has been developed at The University of Nottingham and it has been reported over several papers, [5, 1].

It has been assumed that wave number characterising the microstructure is a Gaussian and isotropic random function. Bearing this in mind, within the parabolic approximation it is possible to obtain a simple expression for second order moment of the acoustic field if the wave number is δ-correlated in the direction of propagation [2]. These assumptions allows significant simplifications in the calculation of the coherence function using phase screen theory. The assumptions may appear too restrictive as grain shape is far more complicated than that but to estimate grain size it may be sufficient. The coherence function from the two points of view are numerically compared as the function using screen theory is too complicated for analytical comparisons. Finally a few experiments were carried out in aluminium to support the above interpretation of aberrations.

PHASE SCREEN APPROXIMATION

In this section, phase screen theory is described to simulate aberrations of ultrasonic waves. A phase screen is a complex number of the form $s = e^{i\phi}$ [4], where ϕ is a random function representing the phase variations of the acoustic field scattered by the grains. The statistical properties of ϕ must be related to the microstructure statistics of the material. Therefore, screens are designed accordingly to the statistical properties of the random wave number in equation (1). In that way it would be possible to calculate the second order moment of the field from two points of view. The random function ϕ is shifting the phase of an incident field v an amount of $\phi = \frac{k_R}{2}\int_0^{\Delta z}\mu(\rho,\zeta)d\zeta$, see [6] and references therein, where μ is a Gaussian zero-mean random function and cross-correlation Γ_μ. In the forthcoming sections we use knowledge of Γ_μ to produce random screens which allows us to simulate ultrasonic field in a random medium. We also assume that ultrasonic waves propagating over the surface of a polycrystalline material can be described by the stochastic Helmholtz's equation which is the basic equation for scalar waves in inhomogeneous random media.

$$\nabla^2 u + k(r)u = 0 \tag{1}$$

here $k = \omega/v_R(r)$ and is being modelled as $k(r,\xi) = k_R(1+\mu(r,\xi))$, where $v_R(r)$ is the velocity and μ is defined above. The relationship between the approximate solution to equation (1) and phase screen theory will be shown. The second order moment or coherence function will be obtained in a separate section as the solution to stochastic equation (1) needs careful explanation. In order to use a phase screen approach the region of interest where the wave is being propagated can be thought of as being divided into several layers of thickness Δz embedded in a homogeneous medium. Each layer represented by a phase screen which randomly shifts the phase leaving the amplitude unchanged. Expanding the acoustic field into plane waves using the angular spectral representation, the acoustic field through a random

screen can be expressed by a random operator defined as

$$\Theta_{\phi,z}[v] \;=\; \int [\frac{1}{2\pi}\mathfrak{v}(p)\otimes\mathfrak{s}(p)]H(x,z-z_0:p)dp \tag{2}$$

where $\mathfrak{v},\mathfrak{s}$ denotes the Fourier transform of $v,s=e^{i\phi}$ respectively. Here, $H=exp[ikz\sqrt{1-p^2}]$ and is a deterministic function acting as a propagator and $\mathfrak{a}=\frac{1}{2\pi}\mathfrak{v}\otimes\mathfrak{s}$ which is the angular spectrum of $v(x)e^{i\phi(x)}$. Let us divide $[0,z]$ into n layers of thickness $\frac{z}{n}$, where n is the number of screens. As a result simulation of aberrations can be carried out by using iteratively Θ, that is $\Theta_{\phi,z}[v] \;=\; \Theta_{\phi,z}[\cdots\Theta_{\phi,z_2}[\Theta_{\phi,z_1}[v]]\cdots]$ or

$$\Theta_{\phi,z}[v] \;=\; \int \mathfrak{a}(q_0)\prod_0^n H(q_j,\frac{z}{n})\prod_0^{n-1}\mathfrak{s}(q_{j+1}-q_j)\exp[ikq_nx]dq_0\cdots dq_n. \tag{3}$$

z's indicates the position each screen is being allocated in space. Equation (3) represents the acoustic field in a random medium and it will serve as a basis to calculate the coherence function. Equation (3) is a multiple integral and we have as many integrals as screens used for the simulation.

By making use of equation (3) it is possible to propagate the coherence function of a plane wave. From now on we distinguish between the coherence function calculated from the phase screen approach, denoted by $\Gamma_{\Theta[v]}$, and the second order moment uf U satisfying equation (1), denoted by Γ_u. The coherence function of the source is denoted by Γ_0.

In principle, it is possible to propagate Γ_0 through one layer and say what exactly $\Gamma_{\Theta[v]}$ is after one screen by directly calculating $\langle\Theta[v]^*(\rho)\Theta[v](\rho')\rangle$. In fact, it would be possible to expect $\Theta[v]$ to be transversally stationary, that is to say $\Gamma_{\Theta[v]}(x-x',z)$ is a function of $\tau=x-x'$ only if the incident field v and screens ϕ are independent in a probability sense. To compute the coherence function at arbitrary points (x,z), (x',z) we have numerically implemented expression (3) and use that information to get the average coherence function. We have an expression for $\Gamma_{\Theta[v]}$ but it was not included in this paper.

PROPAGATION OF CORRELATIONS

Starting from (1) in the parabolic version it is possible to derive a differential equation for the moments of arbitrary order. One important case of this derivation is the second order moment $\Gamma_u=\langle u(x_1,z)u^*(x_2,z)\rangle$ and it can be shown [3, 2], to satisfy the differential equation

$$[ik_R\frac{\partial}{\partial z}+\frac{\partial^2}{\partial u_1\partial u_2}+\frac{ik_R^3}{4}B(u_2)]\Gamma_u(u_1,u_2,z)=0 \tag{4}$$

where $B(x_1-x_2)=T(0)-T(x_1-x_2)$ and $u_1=\frac{1}{2}(x_1+x_2), u_2=x_1-x_2$.

Equation (4) is an ordinary differential equation and its solution can easily be found if statistical properties for μ are assumed and initial condition $\Gamma_0=\langle v(x)v(x')\rangle$. The method to derive equation (4) is to implicitly assume μ to be Gaussian function as the Novikov's formula requires [2]. This formula is the principal ingredient in the derivation of equation (4). Additionally μ has to be assumed δ-correlated in the direction of propagation, that is to say, the correlation function of μ has the form $\Gamma_\mu=\delta(z-z')T(x-x')$. In two dimensions and if μ is an isotropic random function, T and Γ_μ are related by $T(\tau)=2\pi\int\Phi_\mu(w)e^{iw\tau}dw$ where Φ_μ denotes μ spectral density. Thus, if $\Gamma_\mu=\langle\mu^2\rangle e^{-\frac{\tau^2}{a^2}}$ then $T(\tau)=\sqrt{\pi}a\langle\mu^2\rangle e^{-\tau^2/a^2}$. The definition of T involves two parameters mainly $a,\langle\mu^2\rangle$ and also the distance z, where

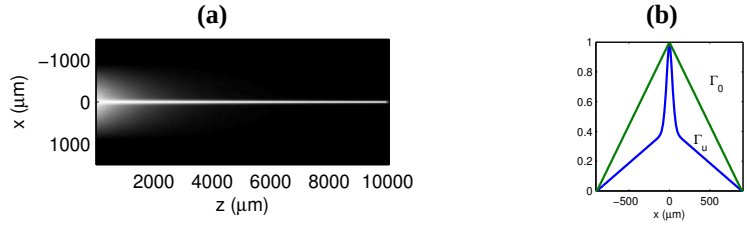

FIGURE 1. (a) Γ_u through inhomogeneous media. (b) Transverse coherence function of image in (a) at the source and at certain distance away form the source.

a is the coherence radius, $\langle\mu^2\rangle$ is a degree of inhomogeneities, respectively. By looking at the general solution to equation (4) we realise that because of the form of $T(\tau)$, Γ_u will be independent of u_1. It is therefore wise to assume from the beginning that $\frac{\partial^2}{\partial u_1 \partial u_2} = 0$; In other words, it can be assumed that the acoustic field u is expected to be a stationary random function. Thereby it is possible to write down a solution for equation (4) in the following form

$$\Gamma_u(\tau) = \Gamma_0 e^{-\frac{\pi^2}{\lambda^2} z(T(0)-T(\tau))}. \tag{5}$$

Here λ is the wavelength of the acoustic field and Figure 1(a) shows an image of Γ_u. The important point in this section is the decay and width of expression (5) which can be seen represented in Figure 1(b), which shows Γ_0 and how it decays away from the source in inhomogeneous medium. The decay is ruled by a and $\langle\mu^2\rangle$ which are chiefly the ingredients for microstructure description. Therefore, the relationship between the coherence function of the field (function that we can measure) and microstructure can be established in simple mathematical expressions in this approximation.

The important value here is $\langle\mu^2\rangle$ which depends on the degree of inhomogeneity and it is related to general behaviour of Γ_u. This asymptotic behaviour is one of the features that the autocorrelation of the acoustic surface field measured from real samples of material shares with this description of ultrasonic propagation. The radius g is defined as the solution to [6]

$$\frac{k^2 z}{4} T(0)(1 - e^{-\frac{g^2}{a^2}}) = 1. \tag{6}$$

The radius g is where the function Γ_u takes small values for $\tau > g$.

Conversely, given the radius of the field g it is possible to obtain the grain size if an approximation for T is used . Specifically, if $T(g) \approx T(0)(1 - \frac{1}{1+\frac{g^2}{a^2}+\frac{g^4}{a^4}})$ then substitution of $T(g)$ in (5) leads to a polynomial equation in a of degree 4 with coefficients in g which can be solved. This calculation may be useful if can be established that the coherence radius of the measured field is truly proportional to grain size. The coherence radius of the field is a quantity that can be measured using the O-SAM instrument.

SIMULATION

In order to simulate aberrations or to generate samples of $\Theta_\phi[v]$ we generate samples of the ensemble ϕ. Taking our definition of ϕ we can generate samples from knowledge of the correlation function Γ_ϕ. Samples for ϕ can be built up in the following way, let $\phi = \int c(\omega) e^{i\omega t} d\omega$ be its Fourier representation for every element in the ensemble where $c(\omega) = \sqrt{S_\phi(\omega)} W(\omega)$, W is white noise process and S_ϕ the power spectrum. Having defined the c's in that way, it is straightforward to corroborate that $\Gamma_\phi(\tau) = \mathscr{F}[S_\phi]$. W being white noise means that W is a Gaussian process with correlation $\Gamma_W = \delta(\omega - \omega')$. W can be easily

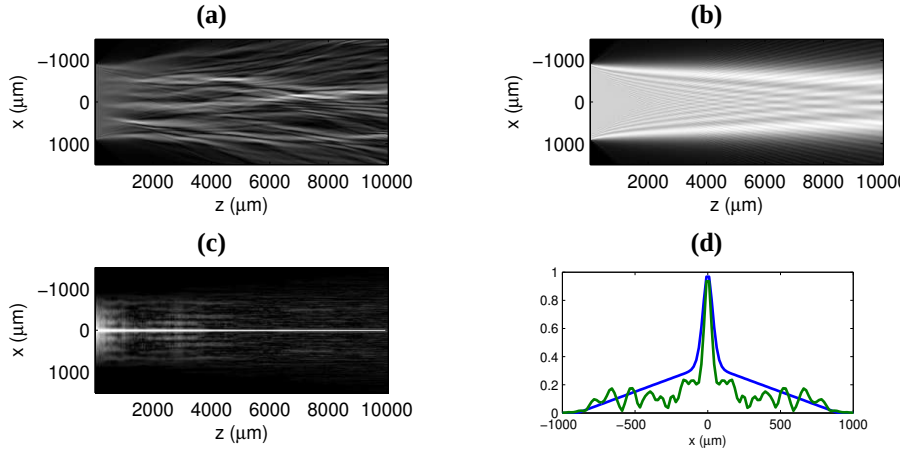

FIGURE 2. Simulation of aberrations in inhomogeneous and homogeneous media (a) and (b), respectively. (a) is a single realisation generated using expression (3). The parameters used for the simulation are $a = 60\mu$m (grain size) and $\langle \mu^2 \rangle = 0.029$ (or 25% velocity variations within the grain). They are roughly corresponding to aluminium. (c) Image of the autocorrelation function calculated numerically from realisation in (a). Averaging those functions we will eventually get $\Gamma_{\Theta_\phi[v]}$ as an average limit function. (d) Comparison of a transverse cross section of $\Gamma_u(\tau)$ and autocorrelation function in (c).

produced numerically. Therefore, in this way, the samples of a random function with known power spectrum are built.

As a consequence, samples for $\Theta_\phi[v]$ can be plotted as it can be seen in Figure 2(a). At this stage we have several ways to obtain the coherence function of the field. Once the realisations of $\Theta_\phi[v]$ has been generated over the ensemble of $k(r,\xi)$ we can calculate the autocorrelation function for a single realisation of $\Theta_\phi[v]$. Figure 2(a) shows a simple realisation of $\Theta_\phi[v](\rho)\Theta_\phi[v](\rho')$ numerically obtained from a single realisation of $\Theta_\phi[v]$. Averaging those functions gives an idea of the mean correlation function with respect to Γ_u when performing the ensemble average $\langle \Theta_\phi[v](\rho)\Theta_\phi[v](\rho') \rangle$. If the number of averaged realisations goes to infinity the ensemble average $\langle \Theta_\phi[v](\rho)\Theta_\phi[v](\rho') \rangle$ will converge to Γ_u. In different words, under same statistics condition $\Gamma_{\Theta_\phi[v]}$ and Γ_u are essentially the same function, compare Figure 1(a) and Figure 2(c). We are also plotting the transverse functions of Γ_u and $\Gamma_{\Theta_\phi[v]}$ away from the source. The graph shows that they are essentially the same.

EXPERIMENTS

The experimental work was carried out in a square piece of aluminium of 30mm×30mm in dimension. The source and detector were positioned at different locations across the

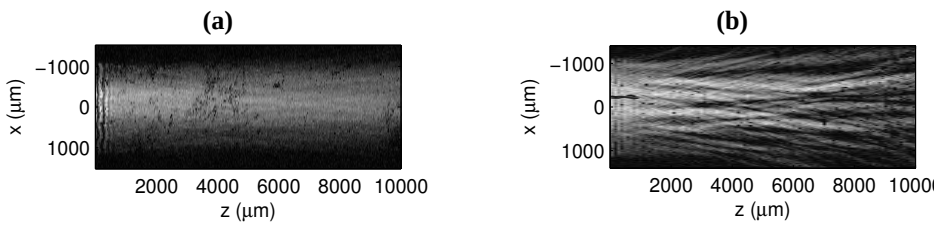

FIGURE 3. (a) Experimental amplitude distribution of the acoustic field of a plane wave travelling in a piece of glass. As glass lacks of grains therefore we get a diffraction pattern (b) Amplitude distribution for aluminium. The amplitude breaks up as the ultrasonic wave travels through the grains producing a speckle patterns. Both images (a) and (b) were obtained with the O-SAM instrument.

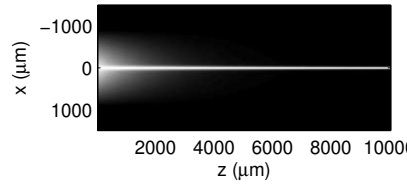

FIGURE 4. Mean coherence function measured on aluminium. This image was obtained by averaging the autocorrelation function over fifty measured speckle patterns on aluminium using the O-SAM instrument. Notice the similarity with Figure 2(c).

whole surface to build up an ensemble of the acoustic field. The autocorrelation function was then calculated for every realisation and ensemble average was obtained numerically to get the mean coherence function for aluminium. The c-scan has been done using the optical acoustic microscope (O-SAM) to detect surface waves. Therefore, with the aid of O-SAM instrument it is possible to show experimental evidence that inhomogeneities or grains cause wave distortions or aberrations to elastic waves. Figure 3(a) is an example of a plane wave propagating from left to right in a homogeneous medium (isotropic glass without inhomogeneities) resulting into a diffraction pattern. Figure 3(b) shows the field amplitude distribution under similar experimental conditions as in (a) but the material is aluminium instead of glass. The amplitude breaks up due to aberration caused by the grain structure. The statistical analysis of speckle pattern obtained is expected to provide some information about microstructure. The size of the grains is proportional to the size of the speckle which correspond to the width of coherence function indirectly calculated from the mean coherence function of the acoustic field in Figure 4.

Some assumptions have to be made for statistical description of the measured speckle. The random function being measured is statistically stationary if not isotropic, i.e. that its transverse autocorrelation function depends on one parameter only. In practise, it is believed that the transverse autocorrelation function will be enough to estimate grain size distribution. Since second order moments or autocorrelation function say how correlated or uncorrelated two points in space are, so the half-width of the transverse autocorrelation will be sufficient to know the grain size. The Figure 5 is $\Gamma_u(\tau, z)$ against the experimental transverse correlation of the function in Figure 4. The three graphs show the functions at $z = 0\mu$m, $z = 5000\mu$m and $z = 8900\mu$m, respectively away from the source.

CONCLUSIONS

We have presented a numerical and an analytical technique to interpret aberrations of ultrasonic waves caused by the microstructure in polycrystalline material like aluminium.

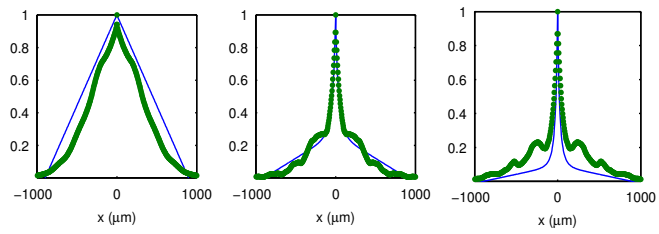

FIGURE 5. Measured transverse coherence function against theoretical Γ_u at three different locations away from the source in a piece of aluminium. The dotted line represent measurements and continuous lines represent theory (Γ_u).

The experimental and theoretical coherence functions have been compared to show that they agree well in the width of central peak, which is proportional to grain size. The coherence function of phase screen theory and stochastic Helmholtz's equation turned out to be physically equivalent. Those two fold approximations allowed us to simulate ultrasonic aberrations due to presence of grains in materials. To give a fairly simple relationship between ultrasonic aberration and grain size. One disadvantage of parabolic approximation is that it neglects backscattering. It seems that there is no way in incorporating backscattering whilst keeping the analytical point of view. The study has to be reviewed to include this process and also more complicated grain structure.

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