Rough surface reconstruction of real surfaces for numerical simulations of ultrasonic wave scattering

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Abstract

The scattering of waves by rough surfaces plays a significant role in many fields of physical sciences including ultrasonics where failure surfaces are often rough and their accurate identification is critical. The prediction of the strength of scattering can be hampered when the roughness is not adequately characterised and this is a particular issue when the surface roughness is within an order of the incident wavelength. Here we develop a methodology to reconstruct, and accurately represent, rough surfaces using an AutoRegressive (AR) process that then allows for rapid numerical simulations of ultrasonic wave rough surface scattering in three dimensions. Gaussian, exponential and AR surfaces are reconstructed based on real surface data and the statistics of the surfaces are compared with each other. The statistics from the AR surfaces agree well with those from actual rough surfaces, taken from experimental samples, in terms of the heights as well as the gradients, which are the two main factors in accurately predicting the wave scattering intensities. Ultrasonic rough surface scattering is simulated numerically using the Kirchhoff approximation, and comparisons with Gaussian, exponential, AR and real sample surfaces are performed; scattering intensities found using AR surfaces show the best agreement with the real sample surfaces.

Keywords:
Ultrasonic wave scattering, Rough surface, Surface reconstruction, Numerical simulation

1. Introduction

Rough surface scattering is important across a broad spectrum of research fields in the physical sciences including optics, electromagnetism, and acoustics, and thus considerable research effort has been devoted to it [1, 2, 3]. The scattered field naturally depends on the incident wave, the medium and the scatterer; typically for smooth planar scatterers the scattering energy is concentrated at the specular angle, however roughness can often have a profound effect with the directivity of the scattered signal spreading to other angles. Roughness is often regarded as decreasing the energy available from the incident waves, since it decreases the reflected, i.e. measured, signal at the specular angle, although conversely the signal increases at other angles;
roughness is often a critical feature of real defects, so modelling based upon smooth scatterers can therefore be misleading.

Rough surfaces form, in their own right, another important research area particularly in solid mechanics and tribology [4, 5, 6]. The accurate characterisation and representation of roughness for two surfaces in contact is an important ingredient when analyzing wear or friction. Surface measurements have historically been limited in accuracy by physical restrictions of measuring tools such as probe sizes or beam widths, and limitations in data storage and computational power hampered the analysis of the data itself. Several parameters have been introduced to describe roughness of a surface, rather than capturing a whole surface measurement, such as the vertical separation of the highest peak and lowest valley [7]. Rapid increases in the development of measuring instruments and computation ability have now ensured that the entire surface can be measured with sufficient sampling density, and statistical descriptions are widely used for explaining rough surfaces [8, 9, 10, 7]. For two dimensional (2D) problems, a surface profile can be described by random heights on a line, and this has been extensively investigated by random process theory originally developed for analyzing time-domain signals [11, 12]; this theory can also describe a random location on the line as well as the random amplitude at the location. For 3D problems, this point process theory has been expanded to allow for data on a surface and this is widely used for image processing which is often entitled as random field theory [13, 14, 15]. The random profile in 2D or the random surface in 3D is often characterised by its Root Mean Square (RMS) of the heights and Auto-Correlation Function (ACF) to describe the amplitude and the texture of random surfaces, respectively.

For a specific application, proceeding directly, a large number of rough surfaces must be obtained, characterised, insonified and the scattered field measured in order to identify the statistics of scattering from that random surfaces. However, it is difficult or sometimes impossible to obtain enough real samples to arrive at statistically reasonable conclusions. One alternative is Monte Carlo (MC) simulation, where a very large number of artificial surfaces are reconstructed and many time-consuming numerical simulations are needed to achieve statistics of wave scattering; much effort has been devoted to increasing numerical simulation efficiency [16, 17, 18, 19, 20]. Although MC studies for wave problems have been largely limited to 2D wave problems [21, 22, 23], these increases in computational efficiency have recently allowed 3D simulation to become feasible for MC simulations [24, 25].

In order to reconstruct surfaces resembling a reference surface, it is often assumed that surfaces are constructed by a linear filtering process with a digital filter. In this case, the filter needs to be modelled or estimated from the reference, and there are several methods to describe the filter. Moving-Average (MA) [26, 27], Auto-Regressive (AR) [28] or Auto-Regressive Moving Average (ARMA) [29] methods are often used for the spectral estimation of the filter. A height at a point is dependant on its neighbouring heights in the AR method, whereas it is on the neighbouring random numbers in the MA method. The MA method is extensively used for surface reconstruction in reflection simulations with Gaussian or Exponential ACF [30, 31, 21, 32, 33, 23], since surfaces can be readily generated relative to AR or ARMA methods. However, the strong relationship between the neighbours in the AR method could result in good estimates of wave reflections since the reflection is dependant on the height gradients as well as the heights themselves.

In this paper, for wave scattering simulations in 3D, we will focus on rough surface reconstruction from real surfaces with particular emphasis on the AR method. The plan of the paper is as follows: In Section 2, the spectral estimation methods for the surface reconstruction are described. Rough surfaces are artificially reconstructed using different reconstruction methods
Figure 1: An illustration for a height $z$ of a rough surface at $\vec{r}$, the location vector of $(i\Delta x, j\Delta y)$ on the region of interest (gray area) on the $xy$ plane. Red solid lines show the cross-sectional profiles of the surface at $x = i\Delta x$ and $y = j\Delta y$. $N_1$ and $N_2$ are the number of grids on the $x$ and $y$ axis, respectively.

and the statistics from each surface group are compared with each other in Section 3. Ultrasonic simulations are executed with the surfaces reconstructed using the Kirchhoff approximation and the results are discussed in Section 4. The paper is summarized and concluded in the last section.

2. Methods to synthesise rough surfaces

In this section, we explain two candidate methods to reconstruct a rough surface: Moving Average (MA) and AutoRegressive (AR) methods. Backgrounds of the surface statistics are provided first, definition of the two methods are described, and then we explain how to estimate the parameters required for the methods.

2.1. General considerations

Rough surfaces can be described by statistics of the heights and the texture or how the heights are scattered across the area of interest [7]. We assume that rough surfaces are defined as a group of heights, $z$, given at regular grid points on $x$-$y$ plane as in Fig. 1. The first and second moments of $z$ are the mean value and the variance, respectively,

$$\mu_z = \langle z \rangle \quad \text{and} \quad \sigma^2_z = \langle z^2 \rangle - \langle z \rangle,$$

where $\langle \cdot \rangle$ means the spatial average over the region of interest. The second moment of the heights becomes $\langle z^2 \rangle$ when $\mu_z = 0$, which is also called the Root Mean Square (RMS) value or more casually roughness [3]. More general statistics of the heights can be expressed using the Probability Density Function (PDF) for the height distribution. The central limit theorem implies the function, for many random signals, becomes the Gaussian distribution:

$$p(z) = \frac{1}{\sigma_z \sqrt{2\pi}} \exp \left( -\frac{z^2}{2\sigma^2_z} \right).$$

The variance and the PDF deal with the amplitudes, and thus contain no indication of surface texture.
Given height amplitude parameters, texture has been investigated using random process theory [34]. The process is characterized by the autocorrelation function, $c_{zz}(\bar{r})$, for surface data $z(\bar{r})$ defined as

$$c_{zz}(\bar{r}) = \frac{1}{N} \sum_{\bar{r}} z(\bar{r})z(\bar{r} - \bar{\tau}) \tag{3}$$

where $N = N_1 \times N_2$ is the number of grid points in the area of interest and $\bar{r}$ indicates a vector from the origin $\bar{0} = (0, 0)$ to grid points $(i\Delta x, j\Delta y)$, or simply $(i, j)$, on the $xy$ plane as shown in Fig. 1. Similarly, the cross-correlation function of two signals, height $z$ and noise $e$ for example, can also be defined as $c_{ze}(\bar{r}) = \sum z(\bar{r})e(\bar{r} - \bar{\tau})/N$. Correlation length ($L_c$) is often used as a proxy for the autocorrelation functions, which is a length where the function decays to $1/\exp(1)$ of its maximal value, within which the statistical relation of surface heights is significant [3].

Another important quantity is the Power Spectral Density (PSD), $S_{zz}$, that describes power distributions over the wavenumber domain of the surface height $z$ and is related to the Fourier transform of $c_{zz}$ as

$$S_{zz}(\bar{k}) = \frac{|Z(\bar{k})|^2}{N} \quad \tag{4}$$

$$= \text{FT} \left[ c_{zz}(\bar{r}) \right] \quad \tag{5}$$

where $\bar{k} = (k_x, k_y)$ is the wavenumber vector, FT$[\cdot]$ means ‘the Fourier transform of’ and the capital letter, for example, $Z(\bar{k})$ denotes the Fourier transform of $z(\bar{r})$. In practice, due to the convenience of the Fast Fourier Transform (FFT), $c_{zz}(\bar{r})$ is frequently computed by Fourier transforming $z$ to get $S_{zz}$ with Eq. (4) and then inverse Fourier transforming the PSD in the view of Eq. (5), rather than by the convolution process in Eq. (3). The cross-PSD is also defined here with the cross correlation function as $S_{ze}(\bar{k}) = \text{FT} \left[ c_{ze}(\bar{r}) \right]$.

### 2.2. Spectral estimation model

A sample of rough surfaces can be described by an output $z$ of a linear filtering process against a random sequence $w$. Surface heights $z(\bar{r})$ are created by convolving the filter $h(\bar{r})$ with the random input $w(\bar{r})$ as illustrated in Fig. 2, and it is expressed as

$$z(\bar{r}) = \sum h(\bar{t})w(\bar{t} + \bar{r}), \quad \tag{6}$$

where the input sequence $w(\bar{r})$ is Independant Identically Distributed (IID) random noise with $(0, \sigma_w^2)$ meaning zero-mean and variance of $\sigma_w^2$ following the Gaussian PDF in Eq. (2), and $h$ is the digital filter having the variance $\langle \hat{h}^2 \rangle = 1/N$. For zero-mean IID random noise $w(\bar{r})$ with
Comparing the above equation with Eq. (6), it is apparent that the equivalent to the filter, 
\[ c_{\text{eq}}(\bar{r}) = \sigma^2_{\text{w}} c_{\text{hb}}(\bar{r}) \quad \text{and} \quad S_{\text{eq}}(\hat{k}) = \sigma^2_{\text{w}} |H(\hat{k})|^2, \]  
where
\[ c_{\text{hb}}(\bar{r}) = \sum_{\bar{t}} h(\bar{t})h(\bar{t} - \bar{r}). \]  
Comparing Eq. (1) and (7) at \( \bar{r} = 0 \), the variance of the input \( w \) is equal to that of the output \( z \) as \( \sigma^2_G = \sigma^2_w \) since \( \sum h^2 = 1 \). The Auto-Correlation Function (ACF) \( c_{\text{hb}} \) is \( c_{\text{eq}} \) normalized by its RMS value and thus it describes the surface texture without considering the absolute value of the heights.

The filter can be described by using Moving Average (MA), Auto-Regressive (AR) or both methods, and they consider the filter as polynomial functionals. The two models will now be briefly explained and their PSD will be derived for the surface reconstruction.

In the Moving Average (MA) process, heights \( z(\bar{r}) \) at a point have linear relation with their neighbouring IID noise \( w(\bar{t} - \bar{r}) \), and thus the random surface can be expressed with its MA parameters \( b \) as
\[ z_{\text{MA}}(\bar{r}) = \sum_{\bar{t}} b(\bar{t})w(\bar{t} + \bar{r}). \]  
Comparing the above equation with Eq. (6), it is apparent that the \( b(\bar{t}) \) in the MA model is equivalent to the filter, \( h(\bar{t}) \), and thus its PSD can be expressed from Eq. (7),
\[ S_{\text{MA}}^{\text{MA}}(\hat{k}) = \sigma^2_{\text{w}} |B(\hat{k})|^2. \]  

The Auto-Regressive (AR) process has the height \( z(\bar{r}) \) linearly correlated with its neighbouring heights \( z(\bar{t} - \bar{r}) \), and is expressed with its AR parameter \( a(\bar{t}) \) as in [29],
\[ z_{\text{AR}}(\bar{r}) = \sum_{\bar{t} \in \Omega} a(\bar{t})z_{\text{AR}}(\bar{t} + \bar{r}) + \sqrt{\nu}(\bar{r}), \]  
where the noise \( e(\bar{r}) \) is a zero-mean sequence and correlated with the AR parameter as its PSD is
\[ S_{\text{AR}}(\hat{k}) = A(\hat{k}) \quad \text{where} \quad A(\hat{k}) = 1 - \sum_{\bar{t} \in \Omega} a(\bar{t})\exp(-i\hat{k} \cdot \bar{t}), \]  
and \( \nu \) is the variance of the noise. Note that the noise \( e \) is not a random IID sequence, unlike the \( w \) of MA model in Eq. (9). However, this introduces an important advantage that the parameters are estimated without iterative computation unlike the estimation of the AR model in time series analysis, the signal is always causal meaning a present signal is only affected by past signals. Its 2D equivalent can be expressed as the summation in Eq. (11) over the area \( \Omega \), not \( (\Omega^- + \Omega^+) \), in that a present height \( z(\bar{r}) \) is affected only by past heights \( z(\bar{t} - \bar{r}) \), not by future ones \( z(\bar{t} + \bar{r}) \). However, for a rough surface, such a constraint does not need to be considered, and thus, in this paper, we use one of the non-causal models from [29].

In order to find the PSD of the AR model, we multiply both sides of Eq. (11) by \( z(\bar{r} + \bar{r}') \) and take their average over \( \bar{r} \), leading to the following equation:
\[ c_{\text{zz}}(\bar{r}') = \sum_{\bar{t} \in \Omega} a(\bar{t})c_{\text{zz}}(\bar{r}' - \bar{t}) + \sqrt{\nu}c_{\text{zz}}(\bar{r}'). \]  
\[ 5 \]
Figure 3: Grid points of interest: $\Omega^+$ and $\Omega^-$ represent future and past area, respectively. Dashed-line area indicates the region for $\bar{r}$, and $\Omega = \Omega^+ + \Omega^-$, the regions for $\bar{r}$, is specified when (a) $\bar{r} = (0,0)$ and (b) $\bar{r} = (1,1)$.

Similarly, multiplying by $e^{i(\bar{r} + \bar{r}')}$ and averaging both sides of Eq. (11) result in

$$c_{zz}(\bar{r}') = \sum_{\bar{t} \in \Omega} a(\bar{t}) c_{ze}(\bar{r}' - \bar{t}) + \sqrt{\nu} c_{ee}(\bar{r}').$$  \hspace{1cm} (14)

Fourier transforming the above equations leads to $S_{zz}^B(\bar{k}) = \sqrt{\nu S_{ze}(\bar{k})/A(\bar{k})}$ and $S_{ze}(\bar{k}) = \sqrt{\nu S_{ee}(\bar{k})/A(\bar{k})}$, respectively, and, by comparing them with Eq. (12), the PSD for the AR model can be obtained as

$$S_{zz}^{AR}(\bar{k}) = \nu/A(\bar{k}).$$  \hspace{1cm} (15)

For the MA or the AR PSDs, their parameters need to be estimated in order to generate rough surfaces or the output $z$, which will be covered in the next section.

2.3. Parameter estimation

The Fourier transform of the MA parameter $b$ can be computed from the PSD of a sample surface $z$ in Eq. (10) with $\sigma_w = \sigma_z$

$$B(\bar{k}) = \sqrt{S_{zz}(\bar{k})/\sigma_z^2}. \hspace{1cm} (16)$$

As can be seen in the above equation, the MA model is rather simple to apply to the surface reconstruction due to the direct relation, and thus the MA method is frequently used for rough surface generation in wave reflection simulations, as mentioned in the Introduction.

The AR parameters can be calculated from the ACF of sample surfaces, but in an indirect manner. We use a non-iterative method following [29] and the method rewritten for the AR method in this section. For further calculations, the correlation function $c_{ze}$ is derived in the view of Eq. (12) as $c_{ze}(\bar{r}) = -a(\bar{r})$ if $\bar{r} \in \Omega + \bar{0}$ with $a(\bar{0}) = -1$, and $c_{ze}$ is obtained by applying the equation to Eq. (14),

$$c_{ze}(\bar{r}) = \begin{cases} \sqrt{\nu}, & \bar{r} = \bar{0} \\ 0, & \text{otherwise} \end{cases} \hspace{1cm} (17)$$

Since we assume that the surface is stationary, the ACF and the AR parameters are thus symmetrical in terms of the origin point, $a(\bar{r}) = a(-\bar{r})$, so that the parameters for $\Omega^-$ are identical to the ones in $\Omega^+$ in the symmetric manner, which will lighten the PSD computation burden. Multiplying $z(\bar{r})$ to Eq. (11) and taking the average over the $r$ lead to the following equation,

$$c_{zz}(\bar{0}) = 2 \sum_{\bar{t} \in \Omega^+} a(\bar{t}) c_{ze}(\bar{t}) + \nu, \hspace{1cm} (18)$$
taking advantage of the symmetry with $c_{zz}(0) = \sqrt{\nu}$ from Eq. (17). The $c_{zz}(\bar{r})$ in Eq. (13) is rewritten with $c_{zz}(\bar{r}) = 0$ from Eq. (17),

$$c_{zz}(\bar{r}) = \sum_{\bar{t} \in \Omega} a(\bar{t}) [c_{zz}(\bar{r} - \bar{t}) + c_{zz}(\bar{r} + \bar{t})],$$

and the summation area for Eq. (19) is indicated, for instance, in Fig. 3 when $\bar{r} = (0, 0)$ and $(1, 1)$.

The AR parameters $a(\bar{t})$ and $\nu$ are found, with surface sample $z$, as follows:

1) Calculate the ACF estimate $c_{zz}$ using Eq. (3),
2) Select the size of the area $\Omega$,
3) Calculate Eq. (19) to get the AR parameters, $a(\bar{t})$, which is computed in its matrix form:

$$[a(\bar{t})] = [c(\bar{r})]^{-1} [c^{-}(\bar{r}, \bar{t}) + c^{+}(\bar{r}, \bar{t})]^T,$$  \hspace{0.3cm} \text{and (20)}

4) Compute Eq. (18) to get the variance of the noise $\nu$ with its matrix equivalent:

$$\nu = c_{zz}(0) - 2[a(\bar{t})][c(\bar{r})]^T,$$  \hspace{0.3cm} \text{where (21)}

$$[a(\bar{t})] = [a(\bar{t}_1) \cdots a(\bar{t}_{m_1})], \quad [c(\bar{r})] = [c_{zz}(\bar{r}_1) \cdots c_{zz}(\bar{r}_{n_1})],$$

$$[c^{+}(\bar{r}, \bar{t})] = \begin{bmatrix}
    c_{zz}(\bar{r}_1 + \bar{t}_1) & \cdots & c_{zz}(\bar{r}_{n_1} + \bar{t}_1) \\
    \vdots & \ddots & \vdots \\
    c_{zz}(\bar{r}_1 + \bar{t}_{m_1}) & \cdots & c_{zz}(\bar{r}_{n_1} + \bar{t}_{m_1})
\end{bmatrix},$$  \hspace{0.3cm} \text{and (23)}

and the superscripts $^{-1}$ and $^T$ mean ‘the inverse of’ and ‘the transpose of’, respectively.

3. Reconstruction of rough surfaces

Rough surfaces are reconstructed based on the method explained in the previous section. A significant step for the reconstruction is to obtain a reference surface, on which the statistics of artificial surfaces are to be based, and, in this paper, a compact tension specimen is used for creating the reference. A number of rough surfaces are generated to resemble the reference surface using the MA and the AR methods, and their statistics are analyzed in this section.

3.1. Generation and measurement of a reference surface

A rough surface sample was generated and its heights were measured as shown in Fig. 4. It was generated with a compact tension specimen of A533B ferritic steel, which is widely-used as a material for pressure vessels. In the generation process, a fatigue crack was first introduced to the specimen and grown with an electro-resonant machine. Secondly, it was torn using a servo-hydraulic test machine, and finally was frozen in liquid nitrogen to be broken apart. Due to the experimental process, the surface is divided into three regions: fatigue, ductile tearing and brittle fracture regions. The surface heights on one half of the specimen were measured using an Alicona optical microscope, and the area measured is approximately $45 \text{ mm} \times 75 \text{ mm}$ with a measuring interval of 50 micrometers.
3.2. Collecting surface samples

In order to take a number of surface samples having similar texture, we selected a part of the brittle region within the red dashed lines in Fig. 4b. From this area, 60 samples of $7.5 \times 7.5$ mm$^2$ square area were obtained, in which neighbouring samples were overlapped for about 66% of the sample due to the limited size of the area; a typical sample is shown in Fig. 4c.

As mentioned in Section 2.1, amplitude and texture are the two main factors which can be used to describe a rough surface. Although the samples are from the same brittle region, some of their statistical characteristics vary one from another, mainly due to low wavenumber components of the surface. In order to guarantee ergodicity or statistical consistency across the samples, we carefully modified the samples as follows.

The data from the surfaces were modified to have zero-mean and zero-tilt. First order polynomial fits were calculated in the least-mean-square manner for each of the samples, and then the tilt-plane components were taken out from the samples so that the samples became zero-mean and zero-tilted surfaces. In Fig. 5, two significant parameters of rough surfaces are compared. Fig. 5a shows the PDFs of the heights before and after the adjustment. The probability distributions without the tilts are consistent relative to ones with the tilts in that they all have zero mean and narrow width across the samples, whereas the original surfaces do not show the ergodic behaviour. The correlation lengths are also compared in the simulations. Before the modifications, the variation of correlation lengths can be clearly seen in Fig. 5b which depend on the collecting locations, but they show fairly consistent character across the ensemble after the tilts are adjusted. The average correlation length in $x$ and $y$ directions are 0.614 and 0.674 mm, respectively, and are used for generating exponential and Gaussian surfaces in the next section.

In addition, the surface roughness was made to be compatible to an input wavelength. For ultrasonic scattering simulation, the roughness needs to be seen by the ultrasonic wave. Thus, the surface heights are increased to have a quarter of the input wavelength for their RMS value, with which simulation results using the Kirchhoff approximation are known to be valid as will be explained more in Section 4, but their correlation lengths are still the same as the red lines in Fig. 5b since only the amplitude of the heights were modified.
3.3. Rough surface reconstruction

In this section, rough surfaces are reconstructed using the MA and the AR methods. Gaussian and exponential surfaces are reconstructed using the MA method, based on the average RMS value and, respectively, the Gaussian and the exponential correlation functions with the average correlation lengths of the 60 samples. AR surfaces are generated using AR methods, based on one sample randomly selected among them.

For the reconstruction, it is convenient to deal with the surface data in the wavenumber domain rather than in the spatial domain, since the wavenumber component is approximately independent and the interpretation of PSD is easier for computation than that of ACF. Once the PSD of a rough surface is designed or acquired, the digital filter \( H(\bar{k}) = \sqrt{S_{zz}(\bar{k})/\sigma_z^2} \) or \( \sqrt{S_{hh}(\bar{k})} \).

Then \( Z(\bar{k}) \) is obtained in the wavenumber domain by \( H(\bar{k}) \times W(\bar{k}) \) from Eq. (6), with a random IID sequence \( w \) of \( (0, \sigma_z^2) \); inverse Fourier transforming generates the rough surface \( z(\bar{r}) \) as

\[
Z(\bar{k}) = \text{IFT}[H(\bar{k})W(\bar{k})].
\]

Two theoretical surfaces, Gaussian and exponential, are generated using the MA model. The ACF \( c_{hh} \) in Eq. (8) of the two surfaces are expressed as \( \exp[-(x/L_x)^2] \) and \( \exp[-|x|/L_x] \) in a 1D profile, respectively [31], as shown in Fig. 6, and notably the correlation length is the only parameter for the function. For 2D surfaces, we select \( x \) and \( y \) direction components, \( L_x \) and \( L_y \), with Gaussian and exponential ACFs respectively:

\[
c_{hh}^{\text{Gau}}(\bar{r}) = \exp[-D^2], \quad c_{hh}^{\exp}(\bar{r}) = \exp[-\sqrt{D^2}],
\]

where \( D^2 = (x/L_x)^2 + (y/L_y)^2 \). The correlation lengths are obtained from the average of ACFs of 60 real samples from Fig. 5b. For the exponential function, we define its shape with elliptic
form as in [35]. For the ACFs being designed, their PSDs can be calculated by their FT from Eqs. (5), and, comparing Eq. (16) and (24), the digital filter $H$ can be directly obtained by Eq. (24). Note that, in estimating MA parameters for the exponential surfaces, the reconstruction procedure mentioned above does not require the artificial offset assumption used in [31], since the surface is calculated in the wavenumber domain.

The AR parameters in Eq. (20) and (21) are calculated from one of the real samples by the procedure described in Section 2.3. The corresponding PSD in Eq. (15) is then ready for the reconstruction, and, from the PSD, the digital filter is computed by Eq. (24). The following is the summary of the procedure for the surface reconstruction:

1) Estimate the $S_{zz}$ from Eq. (10) or (15) via the parameter estimation in Section 2.3,
2) Find $c_{zz}(\bar{0})$ directly or from IFT[$S_{zz}$],
3) Obtain $H$ from Eq. (24) with $\sigma_z^2 = c_{zz}(\bar{0})$,
4) Generate $w \sim (0, \sigma_{ref}^2)$, and its Fourier transform $W$, and
5) Reconstruct the surface $z = \text{IFT}[H(\bar{k})W(\bar{k})]$.

Samples from the different surface groups are shown in Fig. 7. The surfaces look similar to each other except the Gaussian surface which has an apparent smooth texture. However, their statistics will show some differences in the next section.

3.4. Statistics of the surfaces

PDFs of heights and of differences in neighbouring heights from one sample in each group can be seen in Fig. 8. The PDFs of the heights from the surfaces are similar in Fig. 8a, but the PDFs of the slopes have clear differences as shown in Fig. 8b and c. Note that the PDFs of the slopes from the AR surface agree well with those of the real surface in Fig. 8b and c, which shows that the AR method can properly reproduce slopes of a surface. The Gaussian surface shows a very narrow and sharp peak in the figures, meaning that the number of small slopes outnumber those of the larger ones, and thus the surfaces are gradually changing, which is interesting as that is what we observe visually from Fig. 7d. Conversely, the exponential surface has a much broader PDF meaning those surfaces are changing rapidly. These properties
Figure 7: Rough surface samples from the four surface groups: (a) Original sample, (b) AR, (c) Exponential and (d) Gaussian surfaces. Blue and yellow colors represent -0.7 mm and 0.7 mm, respectively.
are to be expected from the shape of their correlation functions at zero, \( C_{hh}(0) \), shown in Fig. 6. Since MA can be seen as averaging the given noises \( w \) with a weighting function related to \( C_{hh} \), the shape of the correlation function at zero determines the sharpness of the surface. The exponential functions are sharp at zero and thus pick up details of the surface, whereas Gaussian functions show smooth shapes and produce somewhat averaged values over the smooth tips. The two synthesised surfaces can be regarded as the two extremes of the real surfaces in terms of the differences between two nearest neighbors, which have a direct influence on the wave reflection, and the results will be covered in Section 4.

For each surface group, 100 surfaces are generated and compared with the 60 real samples mentioned in Section 3.1. Their PDFs in Fig. 9 are similar to those surfaces for the single sample in Fig. 8. We note that the similarity implies that these metrics are ergodic within an identical surface group.

The correlation functions can be calculated from the surfaces. Fig. 10a shows the ACFs of each sample on the x axis, from the four surface groups. In general, the ACFs from the real, the AR and the exponential surfaces show sharp peaks at zero distance and agree well with one another up to the correlation length, indicated by dashed lines, whereas the ACF of the Gaussian surface shows a different shape since the tips at zero are smooth. Beyond the correlation length, the four ACFs show very different configurations. In Fig. 10b, the average ACFs are shown and their behaviours are similar to the ACF with one sample in Fig. 10a up to the dashed line. It can be seen that the average ACFs of exponential and Gaussian surfaces converge to the theoretical ACFs shown in Fig. (6). It is interesting that the average ACF of the AR surfaces fluctuates noticeably even after averaging 100 surfaces. Comparing the pattern of the average ACF of the
Figure 10: Auto correlation function of the sample. (a) ACF of one sample and (b) the average of all the samples, from the real (blue), AR (red), exponential (yellow) and Gaussian (purple) surface groups. Correlation length is the distance at which the ACF becomes 1/exp(1), indicated by (dashed line). The arrows indicate the local minimum and maximum to compare.

AR curves with that of one AR sample, the location of the local minimum and maximum are noticeable both in Fig. 10a and b, as indicated by arrows, and agree well with each other. This feature shows the characteristics of the AR surfaces that the relations between neighbours are very strong because the neighbouring heights are related in a deterministic manner as in Eq. (11).

The correlation lengths are also calculated in the x direction for AR, exponential, and Gaussian surfaces, and the average correlation lengths are 0.510 mm, 0.510 mm and 0.561 mm, respectively, which can be seen from the distance where the dashed line and their correlation functions are intersected in Fig. 10. Provided that the average correlation length of the real surfaces is 0.563 mm, the lengths of AR and exponential surfaces seem to disagree with the real one, but, since it is approximately one sample point difference (≈ 51µm), the effect of the length difference on the texture is insignificant. Comparing the surfaces in Fig. 7, their textures are not enough to be described with a single parameter such as the length, but rather depend on global characteristics of the correlation function.

4. Ultrasonic scattering from the surfaces

In this section, Monte Carlo simulations for ultrasonic scattering from the rough surfaces reconstructed in the previous section are executed using the Kirchhoff Approximation. The approximation is known to be valid when the scattering angle, the surface roughness and the correlation length are in the range of −80° < Θk < 80°, σ < λ/3 and Lx > λ/2, respectively, for Gaussian surfaces [21]. Because the aim of this section is to see the relative comparison with the scattering results, we choose the approximation in order to calculate the scattering efficiently, rather than using more elaborate but time-consuming methods such as finite element method. For the simulations, we choose −60° < Θk < 60°, σ = λ/4 and Lx ≈ λ/2 to have them marginally within the suggested range, since the surfaces considered in this paper are not all Gaussian. A compressive plane wave of 4 MHz is assumed to be incident on the surface with an angle of Θ_in = 0°, and we measure the scattering signals at different directions controlled by Θk and Φ in a steel medium (density: 7800 kg/m³, Poisson’s ratio: 0.2860, and Young’s modulus: 209.3 GPa), whose phase velocity is 5900 m/s and the wavelength is 1.18 mm.
Figure 11: Coordinates for incident and scattered ultrasonic waves. A plane wave is incident with an angle of $\Theta_\text{in}$ whose wave front is parallel to the y axis. The scattered waves are monitored at an angle ($\Theta_\text{R}, \Phi$) on an imaginary hemisphere of radius $|\vec{R}|$. The gray area indicates the location of rough surfaces on the xy plane.

4.1. Numerical simulations

The Kirchhoff approximation corresponds to there being infinitely many flat reflectors following surface slopes located at the surface points [2, 3], and the scattered displacements are calculated by [23] as

$$\vec{u}(\vec{R}) = -i k_\beta \frac{\exp(ik_\beta r)}{4\pi r} \int_{S_m} U_{\alpha\beta} \exp(ik_\beta \varphi_{\alpha\beta}) dS_m \quad \alpha, \beta = p, s$$

where $k_\beta$ is the wavenumber of the wave kind $\beta$, $S_m$ is the surface area, $\vec{R}$ is the vector to a monitoring location from $\vec{0}$ in Fig. 11, $r = |\vec{r}|$, $p$ and $s$ represent the longitudinal and the shear waves and the expressions for the phase $\varphi_{\alpha\beta}$ and the boundary displacement $U_{\alpha\beta}$ can be found in [23] where this approach is extensively investigated. In the scattered fields, gradients of the surfaces play a significant role in the displacements $U_{\alpha\beta}$, and thus the slope of each surface grid becomes important. The intensities of the reflected wave are defined with $\vec{u}$ in Eq. (27) for directions normal to the hemisphere,

$$I(\vec{R}) = |u_x(\vec{R}) \cos \Phi \sin \Theta + u_y(\vec{R}) \sin \Phi \sin \Theta + u_z(\vec{R}) \cos \Theta|^2.$$  

For the 60 real samples and the 100 samples reconstructed for each surface group in Section 3.2 and 3.3, the displacements are calculated by Eq. (27) and their intensities in Eq. (28) are computed 100 mm away from the surfaces, on the imaginary hemisphere as in Fig. 11, with every $5^\circ$ at $\Theta = 0^\circ \sim 60^\circ$ and $\Phi = 0^\circ \sim 360^\circ$. The ensemble average and the Standard Deviation (STD) of the intensities are defined, respectively, as

$$\mu_I(\vec{R}) = \langle I(\vec{R}) \rangle \quad \text{and} \quad \sigma_I(\vec{R}) = \sqrt{\langle [I(\vec{R}) - \mu_I(\vec{R})]^2 \rangle}$$

where $\langle \cdot \rangle$ means ‘the ensemble average of’.

4.2. Scattering Statistics

The average of the intensities relative to the maximum average value from the real surfaces, $\max(\mu_I(\vec{R})_{\text{real}})$, are shown in Fig. 12, seen from the top of the hemisphere. The intensities from
the real samples show several peaks, whereas the other three rarely experience such significant changes across the hemisphere, which is an indication of diffuse wave fields. The fluctuations in the real samples are due to the lack of convergence. Fig. 13a and b show the convergence ratios at the two locations indicated in Fig. 12a. The curve for the real samples at point ‘B’ is not converged yet while the one at point ‘A’ looks to be stable, and, thus in order to achieve a proper average intensity at ‘B’, we ideally need more samples than 60. However, since the average for the reconstructed surfaces are converged, the three groups can be compared. In the figure, the exponential and the Gaussian surfaces look to scatter acoustic energy over the hemisphere, less and more, respectively, than AR surfaces do. In order to compare their overall intensity responses, the spatial average of their intensities are calculated to be 0.233 and 0.511, respectively, compared with 0.396 from the AR surfaces, which shows that the scattering pattern of AR surfaces are between those of the exponential and the Gaussian surfaces.

For fair comparisons with the real surfaces and the artificial surfaces, we select a line of points on the hemisphere (red dashed line in Fig. 12a) at which the results show a good convergence ratio as in Fig. 13a. The average intensities $\mu_I(\mathbf{R})/\max(\mu_I(\mathbf{R})_{\text{real}})$ are shown in Fig. 14a. Results from the AR surfaces agree best with those from the real samples among the three types of surfaces reconstructed. The two curves are located between the results with the Gaussian and the exponential surfaces, which was found when comparing the average intensities in the previous paragraph. At small angles, more specifically, the Gaussian surfaces estimate well the intensities.
Figure 13: Convergence rate of the average intensities at (a) point A, \((\Theta_R, \Phi) = (0^\circ, 0^\circ)\) and b) point B, \((20^\circ, 155^\circ)\), from the real (blue), AR (red), exponential (yellow) and Gaussian (purple) surface groups. Note that the graph for the real surfaces at ‘B’ is still increasing and not converged.

Figure 14: Statistics of the intensities. (a) The average scattering intensities relative to the maximum value from real surfaces and (b) the STD of the intensities relative to the maximum STD, on the dashed line indicated in Fig. 12a, from the real (blue), AR (red), exponential (yellow) and Gaussian (purple) surface groups. The results with the AR surfaces agree best with those with the real surfaces.
from the real ones, whereas the exponential surfaces predict them well at large angles. Therefore, the $\mu_I$ with the two theoretical surfaces can be described as upper and lower bounds at $|\Theta| < 60^\circ$ at least, but it is obvious that they do not accurately reproduce the ultrasonic reflection of the real surfaces. Fig. 14b shows the relative STD of the intensities, $\sigma_I(\bar{R})/\max(\sigma_I(\bar{R})_{\text{real}})$, and the results are similar to the average in Fig. 14a. The ultrasonic simulations show that the results with the AR surfaces look clearly better than the others in their average intensities as well as their STD.

5. Conclusions

We have raised the question of how to accurately reconstruct rough failure surfaces using real surface data in 3D to facilitate the numerical simulation of ultrasonic scattering from rough surfaces. We have reconstructed rough surfaces in 3D using both the MA method with two theoretical correlation functions (exponential and Gaussian) and the AR method based on a reference surface measured by an optical microscope. The AR model is conceptually more powerful as it generates a surface having similar statistics to that of the sample of gradients as well as heights, and a procedure to generate rough surfaces for ultrasonic simulations via AR parameters has been generated. It is encouraging to note that our results show that the PDF of gradients in AR surfaces agrees well with the one from the reference surface, whereas the PDFs from other surface groups are different. Using these surface reconstructions one can naturally try to assess how accurately they then mimic scattering from real surfaces. Wave reflections were also simulated using the Kirchhoff Approximation against the real samples, the exponential, the Gaussian, and the AR surfaces. The average and the standard deviation of scattering intensities from the AR surfaces show the best agreement with those from the real samples among the surface groups considered. In addition, we have found that, relative to real surfaces, Gaussian surfaces provide good estimates at small angles, and conversely exponential ones perform well at large angles, but neither estimate well uniformly across all angles and in some cases the estimates are very poor. Thus we recommend caution be exercised in using results generated by simply assuming that all roughness is characterised by, say, a Gaussian surface. Overall, the statistics from the exponential and the Gaussian surfaces show lower and upper limits in the surface and the scattering intensity statistics considered in this paper. Therefore, to conclude, this study suggests that surface reconstruction using the AR model is most likely to accurately model real samples in terms of their scattering behaviour.

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