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# Simulation of Ultrasonic Materials Evaluation Experiments Including Scattering Phenomena due to Polycrystalline Microstructure

Dascha Dobrovolskij<sup>a†</sup>, Sigrun Hirsekorn<sup>b</sup>, Martin Spies<sup>a†\*</sup><sup>a</sup>Fraunhofer-Institut für Zerstörungsfreie Prüfverfahren IZFP, Campus E3.1, 66123 Saarbrücken, Germany<sup>†</sup>Parts of this work were elaborated at Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, Germany<sup>b</sup>Saarbrücken, Germany

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## Abstract

To evaluate and optimize the performance of ultrasonic inspection and evaluation procedures, we employ the Generalized Point Source Superposition technique (GPSS), which allows to simulate the propagation of ultrasonic waves and their interaction with defects. This contribution reports on the combination of GPSS with the theoretical description of ultrasonic scattering phenomena in microscopically inhomogeneous media. The theory comprises phenomena like local and global directional and position dependent scattering effects in macroscopically isotropic polycrystalline materials. The presented work addresses the main ‘ingredients’ of the simulation procedure and the influence of the grain size on the simulation results.

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*Keywords:* Ultrasound; Simulation; Generalised Point Source Superposition; Scattering Theory

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## 1. Introduction

Simulation methods are increasingly important in the area of non-destructive testing of operational components. To evaluate and optimize the performance of ultrasonic inspection and evaluation procedures, we employ a method based on Huygens’ principle, the Generalized Point Source Superposition technique (GPSS). This technique allows to simulate the propagation of ultrasonic waves and their interaction with defects in media with known material

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\* Corresponding author. Tel.: +49 681 9302 3612; fax: +49 681 9302 11 3612.

E-mail address: [martin.spies@izfp.fraunhofer.de](mailto:martin.spies@izfp.fraunhofer.de)

parameters. Here, we report on the combination of GPSS with the theoretical description of ultrasonic scattering phenomena in microscopically inhomogeneous media, which is of particular interest e.g. for coarse-grained cast materials. The theory comprises phenomena like local and global directional and position dependent scattering effects in macroscopically isotropic polycrystalline materials and provides information about the energy loss due to scattering during ultrasonic wave propagation. To model the grain structure of the material we use the mathematical Point Process approach. This approach generates a geometrical model which represents a close-packed system of cells, which we assume as a fitting model for the polycrystalline material. Due to this geometrical model – called a mosaic - we have statistically distributed points in the three-dimensional space which represent the scattering points. The application of the scattering theory on the material model allows to investigate the energy flux due to the elastic wave forward propagation as well as to the scattering waves separately. To study the interplay of increasing grain size and changes in the ultrasonic frequency we have combined these implementations in a framework called the “Beam Field Simulation Tool”. In this contribution, we address the main ingredients of the simulation procedure and investigate the influence of the grain size on the simulation results.

## 2. Approach and Implementation

### 2.1. Applied Simulation Technique

The GPSS approach exploits the numerical evaluation of a Rayleigh-Sommerfeld-type surface integral where the various physical quantities enter, e.g. the tractions at the transducer surface and the point source directivities in the case of beam field simulation. Similar surface integral representations have been derived for interfaces and scattering surfaces, e.g. defects. In the calculations, equidistant distributions of grid points within the transducer aperture as well as the refracting and scattering surfaces or interfaces, respectively, are used in accordance with the sampling-theorem. As the discretization, i.e. the number of grid points depends on the wavelength, it increases with the transducer frequency. To model transient signals the harmonic (continuous wave) solutions at many frequencies are calculated with a respective frequency spectrum function for the transducer input signal of the probe and then numerically Fourier transformed into the time domain. A detailed description of the method can be found in <sup>1</sup> and <sup>2</sup>.

### 2.2. Scattering Theory

Scattering of ultrasound at microscopic inhomogeneities in materials, e.g. grain boundaries in polycrystals, causes sound velocity dispersion and attenuation. These effects as well as the amplitudes of the scattered waves may be used for materials characterization. Concomitant, scattering at the microstructure of materials hampers defect detection and evaluation because the so-called structural or grain noise superposes the defect signals, and velocity dispersion corrupts the exact defect positioning. This entails the need to include structural scattering into ultrasonic signal analysis and evaluation as well as nondestructive testing simulations.

Numerical simulations of ultrasonic experiments require a convenient microstructural scattering model capable to simulate ultrasonic time signals, e.g. A-scans (backscattering signals), flexible in macroscopic shape and material inhomogeneity (e.g. microstructure variations, defects, etc.) of the considered component, and analytical scattering coefficient formulae allowing fast simulation algorithms. Statistically distributed single scatterers the ensemble averaged scattering energy flux densities of which reflect the grain noise of the test block may be a suitable grain scattering model. Then, the convenient simulation procedure is the GPSS of scattering waves stemming from the scatterers simulating structural noise and in case additionally from defects including possible reflections at the sample surfaces. At the half space surface of a semi-infinite microscopically inhomogeneous solid of macroscopic homogeneity, the GPSS technique will yield the scattering wave intensities well known from the literature.

The solutions of the general equation of motion of inhomogeneous materials contain not only the incident ultrasonic wave and its propagation behavior in the considered medium, but also the scattering waves, i.e. this approach may be exploited for scattering noise computations. Recently, the scattering wave energy flux densities in microscopically inhomogeneous materials are formally derived from the infinite Born series presentation of ultrasonic displacement vectors, the solutions of the elastodynamic equation of motion. The energy flux densities are ensemble averaged respective the microscopic inhomogeneity, evaluated for single phase polycrystals in lowest non-

zero order, correlated to the model simulating grain scattering by statistically distributed single scatterers, and discussed in the context of well-known literature results. A detailed description and literature review is given in <sup>3</sup>. The resultant directional and frequency dependent scattering wave amplitudes are the analytical base for the numerical simulations presented here.

### 2.3. Material Modeling Approach

For modeling the grain structure we use the force-biased algorithm which simulates a random packing of a number of spheres of random diameters without overlapping <sup>4</sup>. Since the scattering theory uses an ensemble statistically averaged over grain orientation and shape and additionally the far-field approximation of the scattering waves, the sphere model to fix the grain structure is convenient. It provides information of the sphere centers and the radii. We consider different realizations  $W_n$  with  $n$  being the number of spheres in a unit cube. Figure 1 shows two realizations of our model with 100 spheres in a unit volume and 30 000 spheres, respectively. The algorithm works with periodic boundary conditions, i.e. the left side-gated spheres of a unit are completed at its right boundary. Thus, the volume and the number of the spheres will give the unit volume fraction filled by spheres:  $c(W_n) = n_{4/3\pi r^3}$  if we assume the radius  $r$  to be constant. We use the software MAVI <sup>5</sup> for the simulation of the sphere packages.

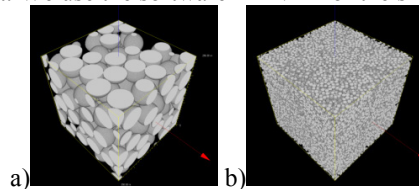


Fig. 1. Sphere packing with a) 100 spheres per unit cube with an estimated radius of 0.1 and  $c(W_{100}) = 0.49$  ; b) 30 000 spheres, estimated radius of 0.01 and  $c(W_{30\,000}) = 0.41$  visualized using MAVI.

### 2.4. Implementation

To combine the material model and the GPSS simulation code we rescale the sphere packages to the region under concern i.e.  $(50\text{mm})^3$ , referring to the simulated beam field in Fig. 2. The summary of the estimated radii is given in Fig. 3, where the star markers flag the sphere packages with discrete number of spheres. For the transducer shown in Fig. 2 generating longitudinal waves we calculate the backscattering coefficients for all sphere centers of one realization. In Figure 3, the backscattering coefficients are shown where bright color indicates large scattering coefficients. The backscattering coefficients become larger due to the increasing scatterer radius and are related to the wave propagation direction, as shown in Fig. 3. In the center of the observed region we see a cone-shaped area with bright colored markers, which means large backscattering coefficient.

## 3. Illustrative Results, Discussion and Outlook

The energy loss due to backscattering is shown in Fig. 4. In the center, the intensity of the propagated elastic wave is high due to the illuminated area by the transducer, thus the outgoing energy shows the highest decrease. The scatterers are marked in this region by dark color. The black markers close to the transducer are lying in its near-field, where the far-field assumption applied in our scattering theory approach does not match. Further results and evaluations of our approach will be published in due course.

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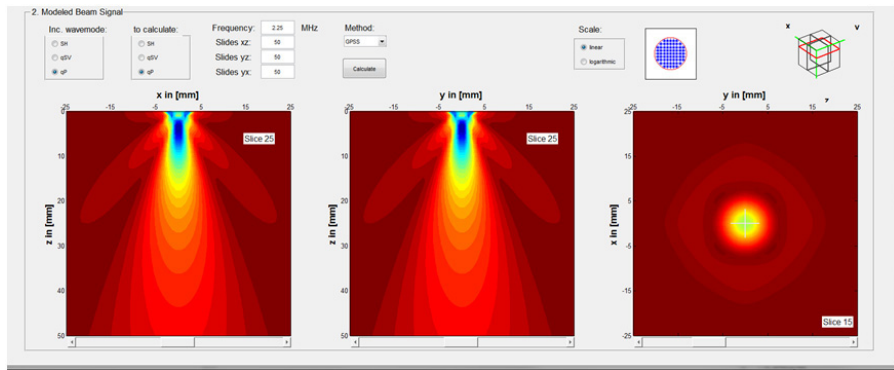


Fig. 2. GUI (developed in MATLAB) with a simulated beam field for polycrystalline nickel with single elastic constants<sup>6</sup>:  $C_{11} = 250 \text{ GPa}$ ,  $C_{12} = 160 \text{ GPa}$ ,  $C_{44} = 118.5 \text{ GPa}$ , density  $\rho = 8.9 \text{ g/cm}^3$ . The beam field is generated by normal incidence L-wave transducer (6.3 mm, 2.25 MHz).

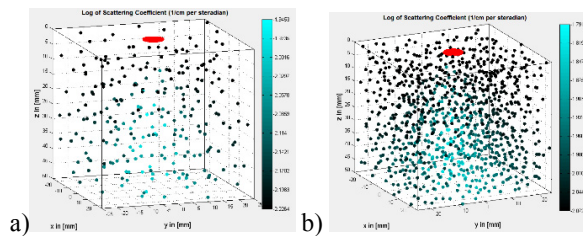


Fig. 3. Visualized are the scattering coefficients for centers of a) 250 and b) 1000 spheres. The red circle indicates the transducer position.

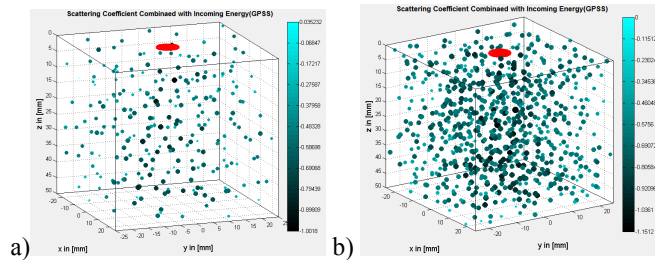


Fig. 4. Visualization of the energy loss due to backscattering for the scatterers' centers of a realization with a) 250 and b) 1000 spheres.

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