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Simulation of ultrasonic structural noise including first and second scattering contributions based on the Born approximation

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Abstract

Structural noise models have several applications in ultrasonic NDE: forward models can help predicting the performances of inspection setups, and inverse models can be used to characterize materials (evaluation of the structure from attenuation and noise simulation/experiment fitting). For polycrystalline materials, an approach based on the Born approximation is widely used in the literature. It has been adapted to various materials and has proven to be particularly accurate for metals such as nickel and titanium alloys. However, its results in the case of strongly scattering metals such as stainless steel used in the nuclear industry have not been fully satisfactory. In this communication, the limits of the Born approximation applied to polycrystalline metals are discussed. A second order Born approximation is proposed as a more accurate alternative. Results are presented and compared to those obtained with other models, in order to highlight the limitations of the first order approximation and the possibilities for improvement. This study has been conducted within the framework of collaboration between IRSN and CEA.

1. Introduction

The scattering of ultrasonic waves by polycrystalline materials creates attenuation and structural noise. These phenomena can be considered difficulties for NDE or means to characterize materials. In both cases, there is interest in their modeling. Earlier models focused on attenuation. Stanke and Kino⁽¹⁾ showed that many of them can be included in a unified theory. These models typically describe polycrystals as an assembly of grains which share the same elastic properties, where scattering occurs because those elastic properties are anisotropic and oriented differently from grain to grain. Models of noise based on the same assumptions have been developed later, many of them following the approach proposed by Rose⁽²⁾. It relies on the Born approximation and only accounts for single scattering. Its validity domain is therefore limited: the Born approximation is known to fail for strong scatterers, and multiple scattering effects are known to be significant in some NDE configurations. However, the exact limits of that validity domain are not easily determined. The work presented in this communication was motivated by the need to assess the applicability of this approach and possible means to improve it, in the context of the modeling of structural noise for some steel components used in the nuclear industry.

In the first section of this communication, the usual application of the Born approximation to the modeling of structural noise is briefly summarized. In the second section, a second order Born approximation is proposed. Finally, results obtained with the different models are compared and discussed.

2. Structural noise in the first order Born approximation

2.1 The Born approximation

The Born approximation, as presented by Gubernatis *et al.*⁽³⁾, can be understood by considering an integral equation that is supposed to be verified by the particle displacement \mathbf{u} in the presence of a scatterer:

$$u_i(\vec{x}) = u_i^{inc}(\vec{x}) + \omega^2 \int_V d\vec{r} \delta\rho(\vec{r}) g_{ij}(\vec{x} - \vec{r}) u_j(r) + \int_V d\vec{r} \delta C_{jklm}(\vec{r}) g_{ij,k}(\vec{x} - \vec{r}) u_{l,m}(r). \quad (1)$$

ω is the angular frequency, V is the volume occupied by the scatterer. $\delta\rho$ and $\delta\mathbf{C}$ the variations of density and of elastic constants compared to the surrounding medium. \mathbf{u}^{inc} is the incident field. \mathbf{g} is the elastodynamic Green function :

$$g_{ij}(\vec{x}) = \frac{1}{4\pi\rho\omega^2} \left[\delta_{ij} k_T \frac{\exp(ik_T|\vec{x}|)}{|\vec{x}|} - \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \left(\frac{\exp(ik_L|\vec{x}|)}{|\vec{x}|} - \frac{\exp(ik_T|\vec{x}|)}{|\vec{x}|} \right) \right]. \quad (2)$$

k_L and k_T are the wave numbers for longitudinal and transverse waves, respectively.

Equation (1) could in theory allow the calculation of the scattered field, but it is generally untractable. However, it allows defining a Born series (a notion first introduced in quantum mechanics) in the following manner:

$$u_i^{N+1}(\vec{x}) = u_i^{inc}(\vec{x}) + \omega^2 \int_V d\vec{r} \delta\rho(\vec{r}) g_{ij}(\vec{x} - \vec{r}) u_j^N(r) + \int_V d\vec{r} \delta C_{jklm}(\vec{r}) g_{ij,k}(\vec{x} - \vec{r}) u_{l,m}^N(r), \quad (3)$$

$$u_i^0(\vec{x}) = u_i^{inc}(\vec{x})$$

The limit of this series for large N is expected to yield the scattered field. What is generally referred to as *the Born approximation* in ultrasonics is simpler, as it is only the first iteration of this series: equation (3) with $N=0$, meaning that the total field in the integral is replaced by the incident field. This will be referred to later in this communication as the first order Born approximation. The next term in the series will be referred to as the second order Born approximation.

Since this approach relies on neglecting the scattered field compared to the incident one, it will be more accurate when the scattered field is small. Practically, this tends to limit its application to weak scatterers, with small sizes and small variations of properties compared to the surrounding medium.

2.2 Application to the modelling of structural noise

In the approach proposed by Rose⁽²⁾, Auld's reciprocity theorem⁽⁴⁾ is applied to a volume of polycrystalline material. An expression of the signal backscattered by a polycrystalline material is obtained. In a monophasic polycrystal, the signal S at angular frequency ω can be written:

$$S(\omega) = \frac{1}{i\omega} \int_V d\vec{x} \delta C_{ijkl}(\vec{x}) u_{i,j}^{incEm}(\vec{x}) u_{k,l}^{totRe}(\vec{x}). \quad (4)$$

δC is again the variation of elastic constants, though this variation is now defined with respect to the average elastic constants in the polycrystal. It is an average over grain orientations since grain orientations are assumed to be the only reason elastic properties differ from grain to grain.

Following Auld's framework, the displacement field \mathbf{u}^{incEm} is the field that would be generated by the emitter in the absence of scatterers, meaning the incident field from the emitter. Since the scattering is due to the inhomogeneity of the material, the ultrasonic field in the absence of scatterers is the field that would propagate in a homogeneous averaged medium. \mathbf{u}^{totRe} is the total field that would be generated if the receiver acted as an emitter and the scatterers were present.

Like equation (1), equation (4) expresses scattering as a function of an integral over an untractable total field. The first order Born approximation replaces it by the incident field and yields:

$$S_{Born1}(\omega) = \frac{1}{i\omega} \int_V d\vec{x} \delta C_{ijkl}(\vec{x}) u_{i,j}^{incEm}(\vec{x}) u_{k,l}^{incRe}(\vec{x}). \quad (5)$$

\mathbf{u}^{incRe} is the incident field (i.e the field in the absence of scatterers) from the receiver. Equation (5) allows calculating the structural noise signal if the incident field is known. It also allows calculating quantities that characterize the tendency of a material to generate structural noise. Margetan *et al.*⁽⁵⁾ define a coefficient η that quantifies the average intensity scattered by a unit volume of the microstructure. They give its analytical expression for all modes and directions. The term Figure Of Merit (FOM) is also sometimes used in the literature to refer to another coefficient that gives the same information. The expressions obtained for these coefficients based on the approach presented here depend on elastic properties and grain sizes.

2.3 Validations and applications

Such coefficients were measured and calculated by Thompson *et al.*⁽⁶⁾ as an early verification of Rose's approach. They tested three materials: alpha-titanium, copper, and 304 stainless steel. Their theoretical and experimental ranges for these coefficients were in agreement in the case of titanium and copper. However, the coefficient they measured for steel was significantly higher than what the model predicted.

Later, other authors used the same model in inversion procedures to deduce grain sizes from ultrasonic noise. For example, Panetta *et al.*⁽⁷⁾ were successful in determining grain sizes in some nickel alloys based on noise measurements.

The model has also been used for computations of structural noise in NDE simulation. Dorval *et al.*⁽⁸⁾ proposed a simulation method and tested it by simulating measurements performed on steel samples. The simulated noise they obtained was underestimated compared to measurements, which is reminiscent of the early results obtained by Thompson *et al.*⁽⁶⁾ for steel.

A pattern seems to emerge where the model is more accurate for some materials than for others. Since the Born approximation is supposed to be most suited for weak scatterers, it could be that its application to polycrystal works best for materials with low variations from grain to grain, meaning with low grain anisotropy.

Results presented by Hu and Turner⁽⁹⁾ seem to support that explanation. They developed a model that includes double scattering and presented computations for two materials: aluminium (weakly anisotropic) and iron (highly anisotropic). They obtained significant double scattering contributions only for iron. Since the first order Born approximation only include single scattering, their results would imply that it is significantly less accurate for iron than for aluminium.

That context motivated the development of the second order Born approximation presented below. It was expected to correct some of the inaccuracies of the usual Born approximation for highly scattering material, and to include some double scattering.

In order to allow comparisons with results obtained by other authors, it will be tested for materials previously considered by Thompson *et al.*⁽⁶⁾ (limited to their materials with cubic crystallographic symmetry, since others are not implemented yet in the approach presented here) and by Hu and Turner⁽⁹⁾. These properties are summarized in Table 1.

Table 1. Properties of the tested materials

Material	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	A (GPa)	ρ (g/cm ³)	v_{0L} (m/s)	v_{0T} (m/s)
Copper ⁽⁶⁾	169	122	75.3	-103.6	8.89	4865.34	2477.80
Stainless steel ⁽⁶⁾	216	145	129	-187	8.12	5984.38	3358.69
Aluminium ⁽⁹⁾	106.7	60.41	28.34	-10.39	2.7	6407.63	3118.76
Iron ⁽⁹⁾	219.2	136.8	109.2	-136	7.86	5922.58	3242.35

A is an anisotropy factor, v_{0L} and v_{0T} are velocities for a Voigt averaged medium. They are calculated as a function of the other parameters:

$$\begin{aligned}
 A &= C_{11} - C_{12} - 2C_{44}, \\
 v_{0L} &= \sqrt{\frac{3C_{11} + 2C_{12} + 4C_{44}}{5\rho}}, \\
 v_{0T} &= \sqrt{\frac{C_{11} - C_{12} + 3C_{44}}{5\rho}}.
 \end{aligned} \tag{6}$$

3. Second order Born approximation

3.1 Development of the approximation

The expression of structural noise in the first order Born approximation (5) was obtained by substituting the total field with the incident field in equation (4). To go one order higher, it will be substituted instead with the next term in the Born series (3). Density variations are omitted since none exist for the polycrystals considered. The following expression is obtained:

$$S_{Born2}(\omega) = \frac{1}{i\omega} \int_V d\vec{x} \delta C_{ijkl}(\vec{x}) u_{i,j}^{incEm}(\vec{x}) \left[u_{k,l}^{incRe}(\vec{x}) + \int_V d\vec{r} \delta C_{abcd}(\vec{r}) g_{ka,bl}(\vec{x} - \vec{r}) u_{c,d}^{incRe}(\vec{r}) \right]. \quad (7)$$

Double scattering appears in equation (7): ultrasonic waves first travel from the emitter to \mathbf{x} with $u_{i,j}^{incEm}(\vec{x})$, and interact with the microstructure at \mathbf{x} . Then, a part travels directly to the receiver with $u_{k,l}^{incRe}(\vec{x})$. Another part travels from \mathbf{x} to \mathbf{r} with $g_{ka,bl}(\vec{x} - \vec{r})$, and interacts there before traveling to the receiver with $u_{c,d}^{incRe}(\vec{r})$.

Unlike equation (5), equation (7) does not allow for simple analytical evaluations. A numerical approach was implemented. The terms depending on \mathbf{x} and \mathbf{r} are evaluated at coordinates placed on a regular 3D grid. The grids for \mathbf{x} and \mathbf{r} have an offset of a half step relative to one another in order to avoid the case $\mathbf{x}=\mathbf{r}$, which causes a singularity of the Green function. The integrals are calculated using a Riemann method. The approach has a computational cost that grows proportionally to N^6 , N being the numbers of point of the grids for a given coordinate and N^3 their sizes. As a consequence, N will be kept low.

3.2 Application to a canonical problem

As a validation, outputs of this approach were compared to a reference solution for the canonical problem of the scattering by a spherical inclusion. The reference solution is an exact expansion based on a separation of variables (SOV), described for example by Brill and Gaunard⁽¹⁰⁾.

For plane waves of amplitudes u_0^{incEm} and u_0^{incRe} , with v_{Re} the velocity of the wave considered in reception, a scattering coefficient D can be defined based on equation (4):

$$D = \frac{1}{4\pi\rho v_{Re}^2 u_0^{incEm} u_0^{incRe}} \int_V \delta C_{ijkl}(\vec{x}) u_{i,j}^{incEm}(\vec{x}) u_{k,l}^{totRe} d\vec{x}. \quad (8)$$

This coefficient has been evaluated for spherical inclusions using the SOV approach and the first and second order Born approximations. Both Born approximations were

evaluated numerically using the regular grid described in the previous section. An analytical expression can also be obtained for spheres in the first order Born approximation⁽³⁾: it was included in the comparisons in order to get a sense of the error introduced by numerical calculations. To test their ability to yield acceptable results while limiting computation times, the numbers of points of the grid were chosen to be relatively low. The \mathbf{x} and \mathbf{r} grids used are cubes with a width equal to the sphere diameter and $20*20*20$ points.

Figure 1 shows examples obtained for two spherical inclusions of radius R . The surrounding medium has isotropic properties based on the steel of Table 1. The velocities v_{IL} and v_{IT} in the spheres have been set to be slightly different from the surrounding medium. k_{0L} is the wave number associated to the velocity v_{0L} .

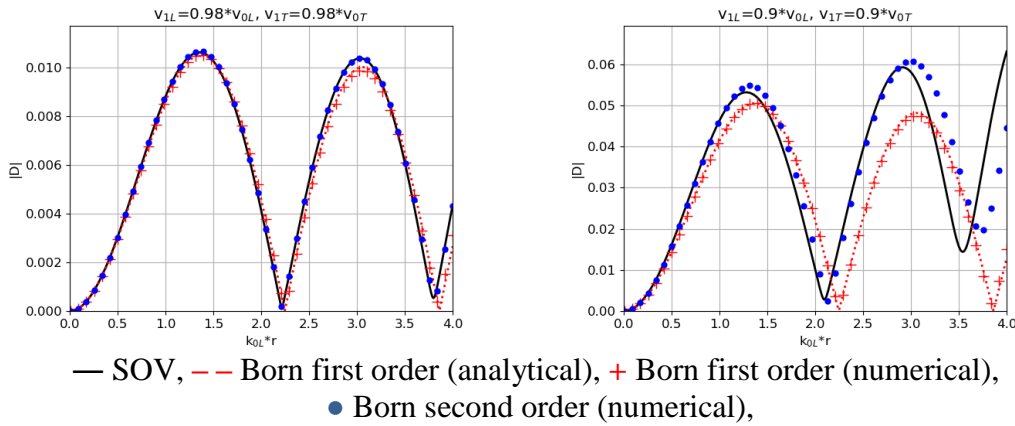


Figure 1. Scattering coefficient as a function of $k_{0L}*R$ for spheres in steel

These results do not exhibit any problems that could be caused by the numerical approach: analytical and numerical results for the first order approximation are very close, and no aberration appears in the second order numerical results either.

The two results of that figure correspond to two different materials. The first one has a very weak contrast compared to the surrounding material and the second one a slightly higher one. As expected, both orders of the Born approximation appear to be more accurate for lower contrasts and lower $k_{0L}*R$. Its second order is confirmed to be closer to the reference than its first order. It is not exactly equal to the reference, especially for higher contrast, but still significantly reduces the error.

4. Comparisons of results for polycrystals

4.1 Scattering by a single crystal

As Figure 1 shows, the second order of the Born approximation modifies and improves the calculation of scattering even for an isolated scatterer. Before applying to a polycrystal where interactions between several grains will be taken into account, its effects on a single isolated crystal are examined. Figure 2 shows results obtained with the two Born approximations for a single crystal. Its geometry is from a grain of one of the polycrystals presented afterwards, its volume is noted V , and its elastic properties

were obtained by randomly determining orientations. The three results shown are a sample of the behaviour observed for different orientations.

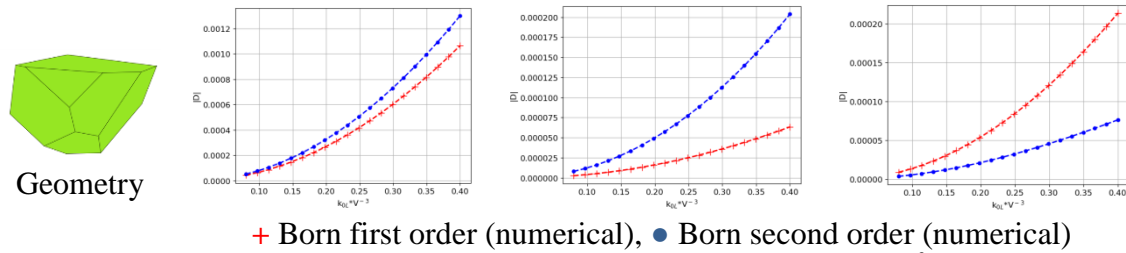


Figure 2. Examples of scattering coefficients as a function of $k_{OL} * V^3$ for an isolated steel crystal

In these examples, like in other tests performed not presented here, the outputs of the two models seem to differ mainly by a constant multiplicative factor. This factor is not the same for different orientation. In most cases the second order approximations yields larger coefficients, though not always.

The results presented for polycrystals in the next section will be different because they will include the effects of an averaging over a set of grain shapes and orientation. In the case of the second order approximation, they will also include some double scattering effects involving neighbouring grains.

4.2 Application to scattering by polycrystals

Average scattering coefficients for polycrystals can be obtained analytically in the first order Born approximation. It is also possible to obtain them numerically by generating examples of polycrystals.

Polycrystals were represented using Voronoi diagrams. They were calculated for random points in a cubic volume following a uniform distribution. It was ensured that the diagrams fit exactly in a cube by placing symmetrical points outside of it. All the results presented here were obtained for diagrams with 50 cells. Examples are shown Figure 3.

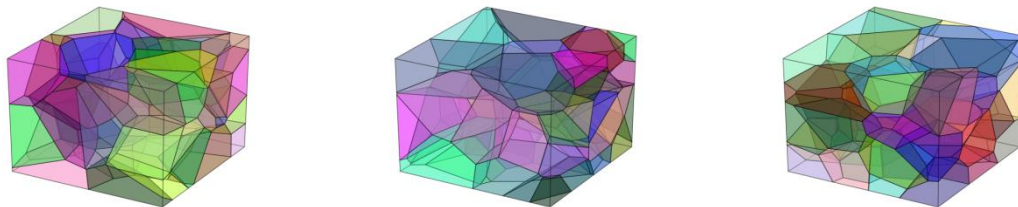


Figure 3. Examples of Voronoi diagrams used for noise calculations

Each Voronoi cell is treated as a grain and a random orientation is assigned to it. Its elastic constants are determined by that orientation.

For each polycrystal, the structural noise signals were computed at a given frequency in the first and second order Born approximations based on expressions (5) and (7). The average backscattering coefficients η , as defined by Margetan *et al.*⁽⁵⁾, can be obtained by averaging the intensity of the calculated signals and normalizing them by the intensity of incident waves and the volume considered.

These coefficients were also calculated analytically in the first order Born approximation. However, their usual expression is not exactly suited to Voronoi diagrams. It depends on a spatial correlation function, defined as the probability that two points fall in the same grain. It is usually assumed to behave as a decreasing exponential function of the distance between the points, which is not entirely accurate for Voronoi diagrams. A spatial correlation function for the Voronoi diagrams can nonetheless be calculated and allows computing suitable coefficients⁽¹¹⁾.

For each of the four materials of Table 1, computations were performed for 150 examples of polycrystals at several $k_{0L} \cdot V_{av}^{-1/3}$, V_{av} being the average volume of a grain. The emitted and received waves considered were longitudinal plane waves propagating in the same direction, simulating a configuration where the same probe is used as emitter and receiver. Results are presented in Figure 4. Since the numerical coefficients are obtained by averaging random results, confidence intervals can be calculated and are also plotted.

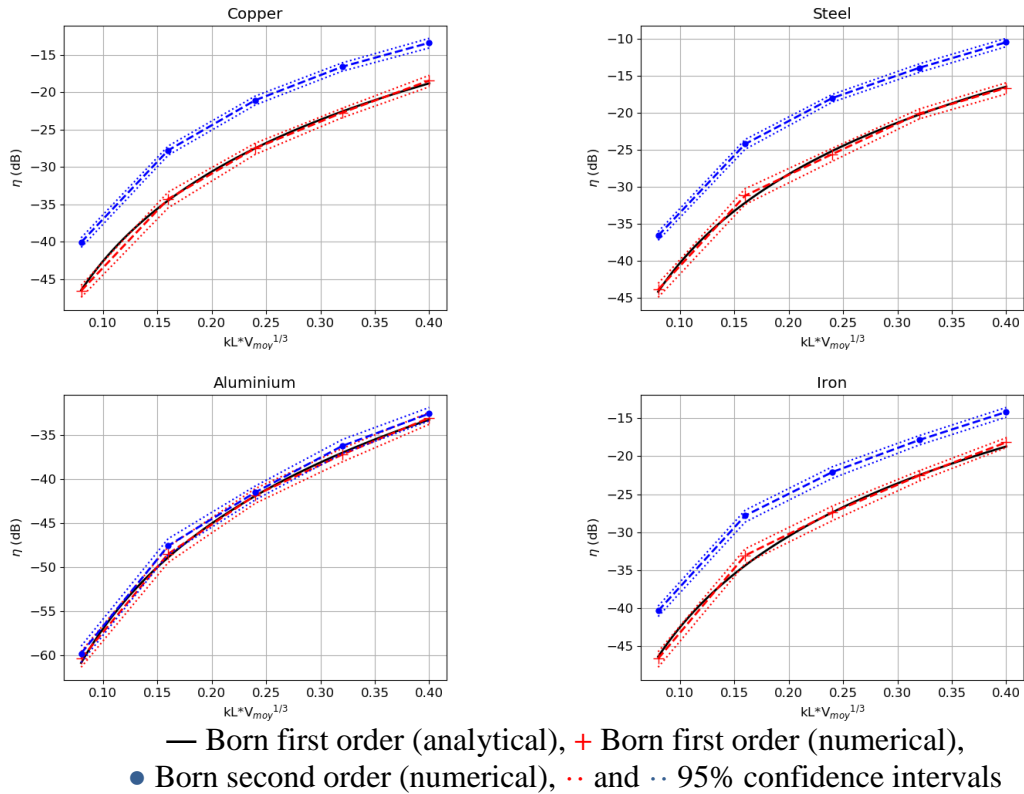


Figure 4. Average scattering coefficients of polycrystals as a function of dimensionless wave number

Analytical first order coefficients fall in the confidence interval of their numerical counterparts, confirming that the two calculation methods are equivalent.

Contrary to those of Figure 1 and Figure 2, the results are presented in decibels. It emphasizes the fact that there seems to be a multiplicative factor between the results of the two approximations, and that this factor does not vary significantly with frequency. The averages of the corresponding decibel offset are given in Table 2 for readability.

Table 2. Average offset between single and double scattering calculations

Copper	Steel	Aluminium	Iron
6.1 dB	6.8 dB	0.7 dB	5.1 dB

The stability of that offset with frequency is consistent with the behavior observed in Figure 2. However, it was not entirely expected since it differs from the double scattering results obtained by Hu and Turner⁽⁹⁾. For aluminium, they find no significant contributions for double scattering, which is consistent with what is observed here. However, for iron, their doubly-scattered results are very similar to the single-scattered ones for $k_L \cdot D$ equal to 0.08, slightly higher for 0.16 and more than double for 0.32. In Figure 4 there is an almost constant and significant offset at those three wave numbers. Since their model and the one presented here are different, it might be that they do not account for the same phenomena. The offset obtained here could mainly be a correction of the scattering by single grains, such as the one observed in Figure 4. Double scattering could be expected to add itself to that offset and to increase the gap at higher wave numbers. It is not the case here, and it might be because the calculations were done for a small volume of grains where possibilities of double scattering are limited.

Regardless of the cause of the offset, the results of Table 2 suggest that the first order Born approximation has significant inaccuracies for several materials. In particular, the offset obtained for steel would explain the underestimation observed by Thompson *et al.*⁽⁶⁾ and by Dorval *et al.*⁽⁸⁾ with the first order approximation. The case of copper is more surprising, as Thompson *et al.* had obtained a good agreement between theory and experience. However, that agreement might have been due to the wide range of coefficients they accepted as correct due to uncertainties concerning grain sizes. The case of aluminium confirms that the first order Born approximation can be safely applied to weakly anisotropic polycrystals.

5. Conclusion and perspectives

Adding a second order to the Born approximation provided significant insight concerning its validity. It confirmed that its application to the modeling of structural noise can be more or less accurate depending on the material. It also suggests ways to improve these models. Though one of the motivations of these developments was to include effects of double scattering, the results obtained indicate that another phenomenon is significant: the first order Born approximation can cause significant errors even in the computing of the scattering by single grains of strongly anisotropic materials.

The second order Born approximation calculations presented here are at the moment limited to equiaxed and non-textured materials with cubic crystallographic symmetries, and to backscattering of longitudinal waves. Some adaptations are necessary in order to generalize it to more materials and measurement setups.

It is a computationally intensive approach and cannot readily be integrated in simulation tools for industrial applications. Several options are being considered to allow it. It might be possible to do at least a part of the calculations analytically, reducing the numerical cost. Another possibility would be to use the results of the numerical model as a reference in the development of a simplified and fast approach whose error would be controlled. It would also be possible to use a data base of outputs of the numerical model to quickly calculate scattering coefficients by interpolation.

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