

GRAIN-BOUNDARY SCATTERING OF SURFACE ACOUSTIC WAVES: EXPERIMENT, THEORY, AND SIMULATION

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Outline



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- Grain-Boundary Scattering of Longitudinal Bulk Waves
- Grain-Boundary Scattering of Surface Acoustic Waves

FEM simulation of L-wave scattering

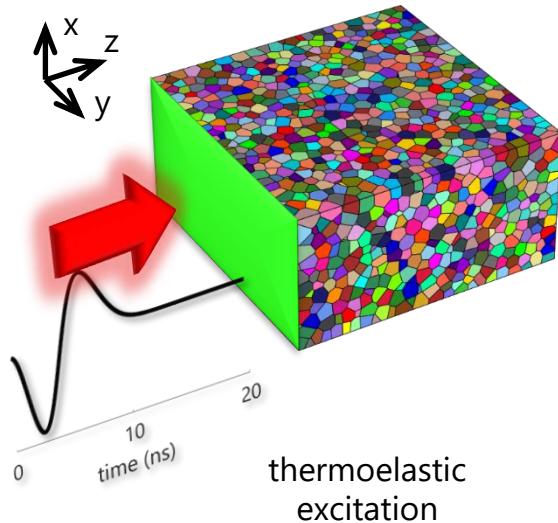


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[M. Rzy et al., J. Acoust. Soc. Am. 143, 219 (2018)]

- Virtual polycrystal: Voronoi tessellation
- Time-domain FEM simulation of L-wave propagation

Tessellation Software: Neper
FEM Software: PzFlex



8000 grains
 $1 \times 2 \times 2 \text{ mm}^3$

375 mil. DoF (12 runs)
el. size $3.2 \mu\text{m}$, time step 0.4 ns

FEM simulation of L-wave scattering

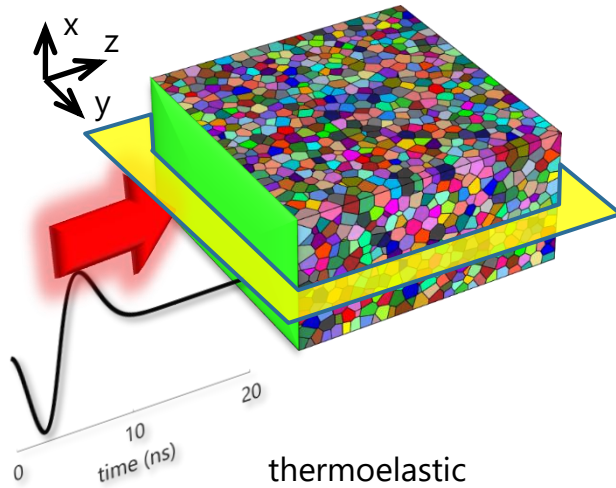


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[M. Rzyz et al., J. Acoust. Soc. Am. 143, 219 (2018)]

- Virtual polycrystal: Voronoi tessellation
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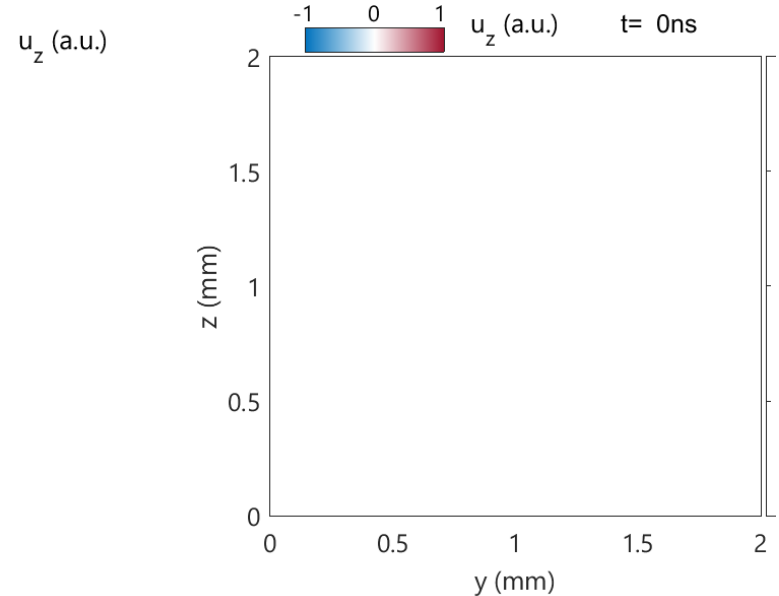
Tessellation Software: Neper
FEM Software: PzFlex



thermoelastic
excitation

8000 grains
 $1 \times 2 \times 2 \text{ mm}^3$

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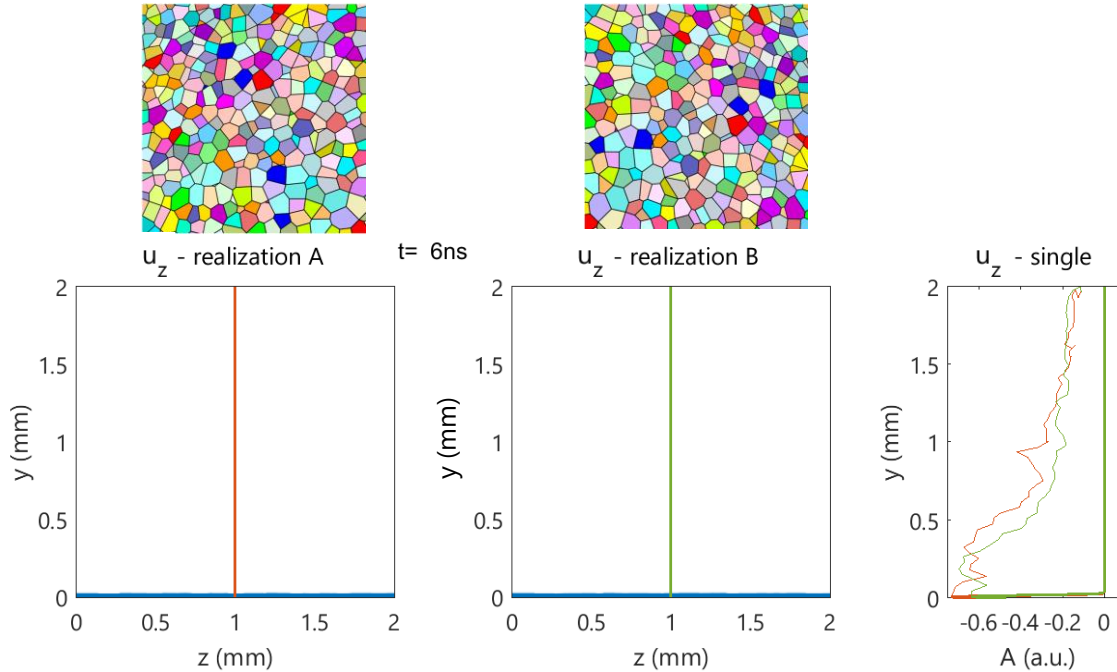


Time-domain FEM simulation of
longitudinal-wave propagation

Coherent wave and attenuation



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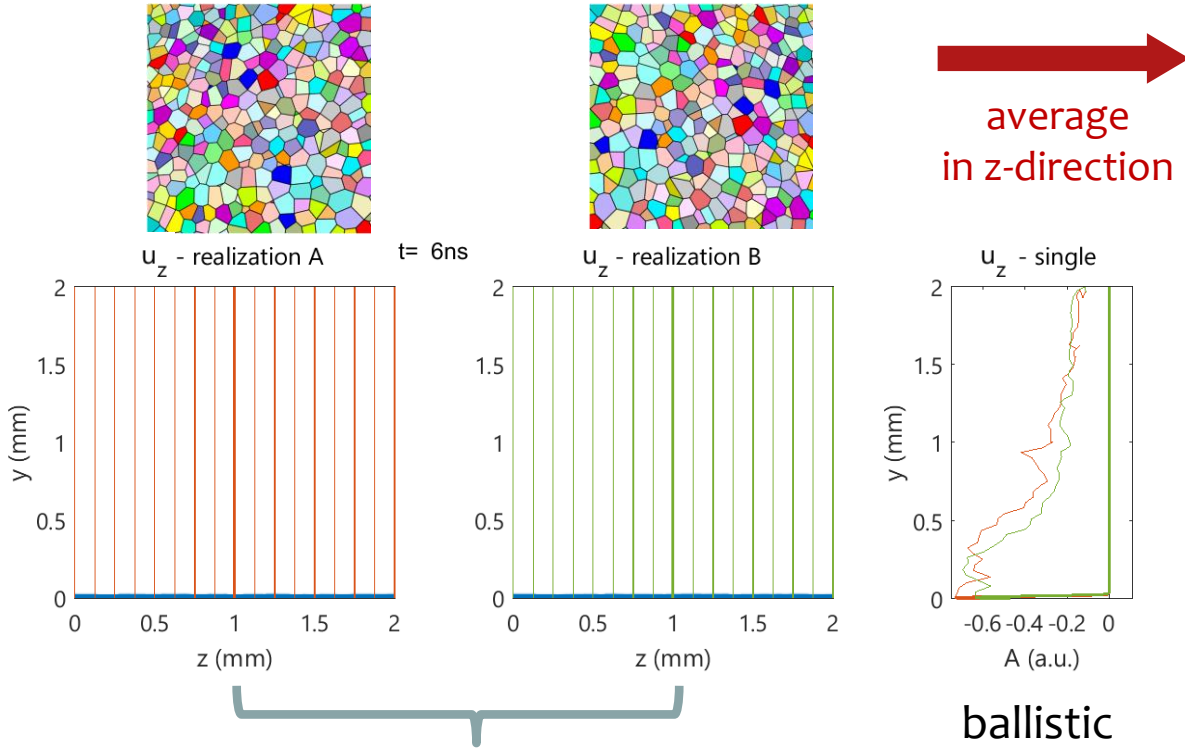
Same statistics (e.g. mean grain \emptyset),
different microscopic realization

ballistic
wave

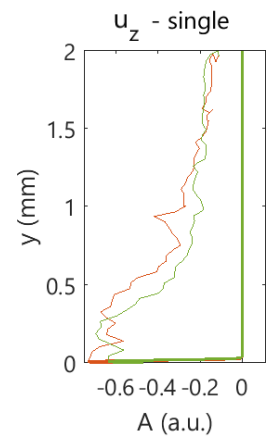
Coherent wave and attenuation



6



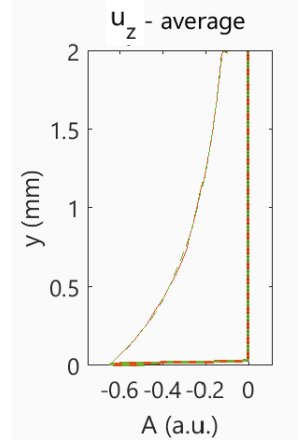
average
in z-direction



ballistic
wave

Attenuation

- Macroscopic
- Effective medium



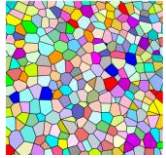
'coherent wave'

Same statistics (e.g. mean grain \emptyset),
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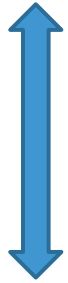
Coherent wave and attenuation



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Polycrystal
 $\tilde{u}(x, \omega) = ?$



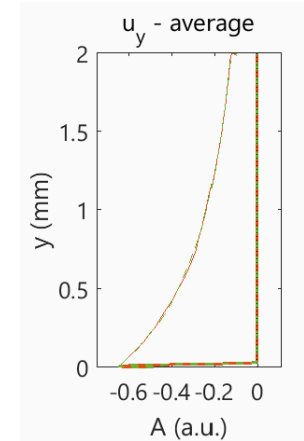
Coherent wave $\langle \tilde{u} \rangle(x, \omega) \propto e^{i(\tilde{k}x - \omega t)}$

$$\frac{\omega}{c(\omega)} + i\alpha(\omega)$$



Effective *homogeneous* medium
with only parametrical description
of the microstructure

- Attenuation
- Macroscopic
 - Effective medium



'coherent wave'

Scattering Regimes & Asymptotes



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- Relation between attenuation $\alpha(\omega)$ and *microstructure* (grain size d)?

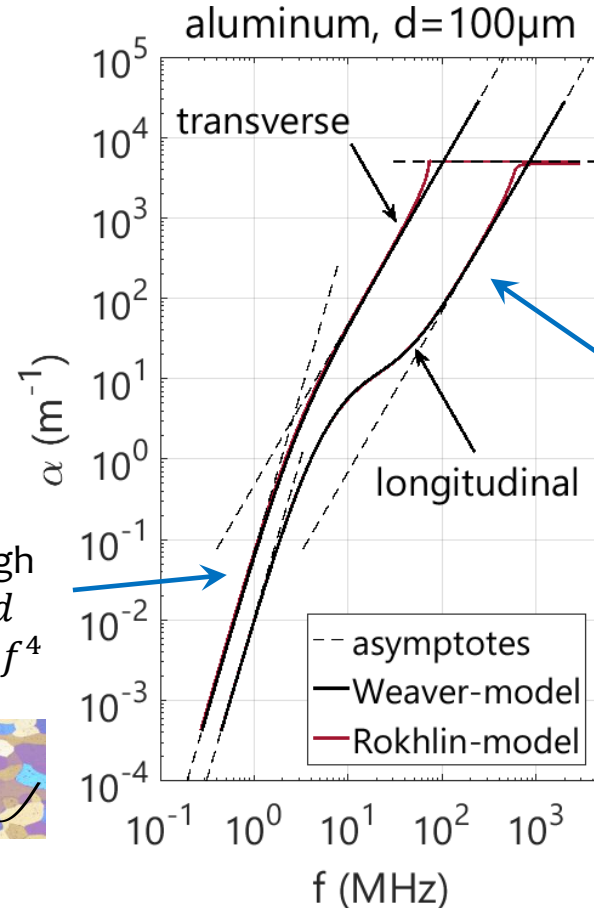
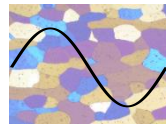


Analytical
(attenuation)
model

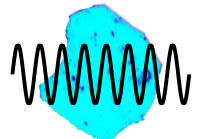
e.g.: Weaver's model

[Weaver, *J. Mech. Phys. Solids* 38 (1990)]

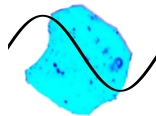
Rayleigh
 $\lambda \gg d$
 $\alpha \propto d^3 f^4$



geometric
 $\lambda \ll d$
 $\alpha \propto \frac{1}{d}$



stochastic
 $\lambda \approx d$
 $\alpha \propto d f^2$



Simulation vs Experiment

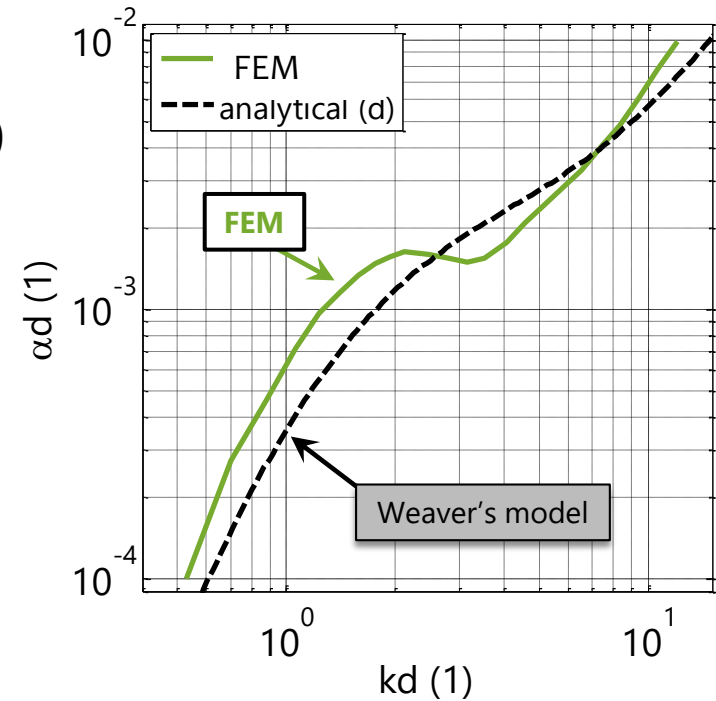


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[M. Ryzy et al., J. Acoust. Soc. Am. 143, 219 (2018)]

- Weak agreement with the model
 - ▣ Microstructure description?
 - Mean grain size d
and assumed two-point correlation function (TPCF)

$$w(r) = e^{-r/d}$$



Simulation vs Experiment



□ Weak agreement with the model

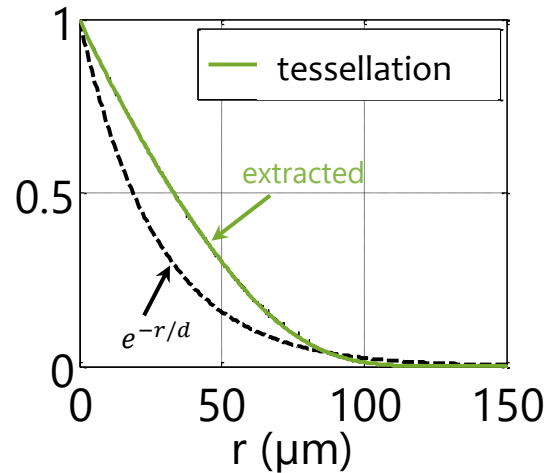
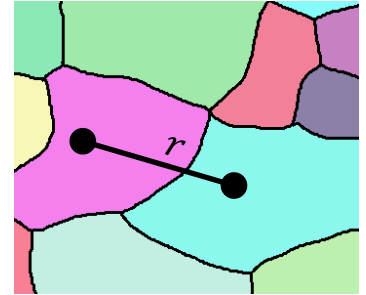
▣ Microstructure description?

■ Mean grain size d
and assumed two-point correlation function (TPCF)

$$w(r) = e^{-r/d}$$

■ Not in agreement with
the TPCF of the tessellation!

Two-point correlation function:
the probability that two points
separated by r are within the
same grain



Simulation vs Experiment



□ Weak agreement with the model

▣ Microstructure description?

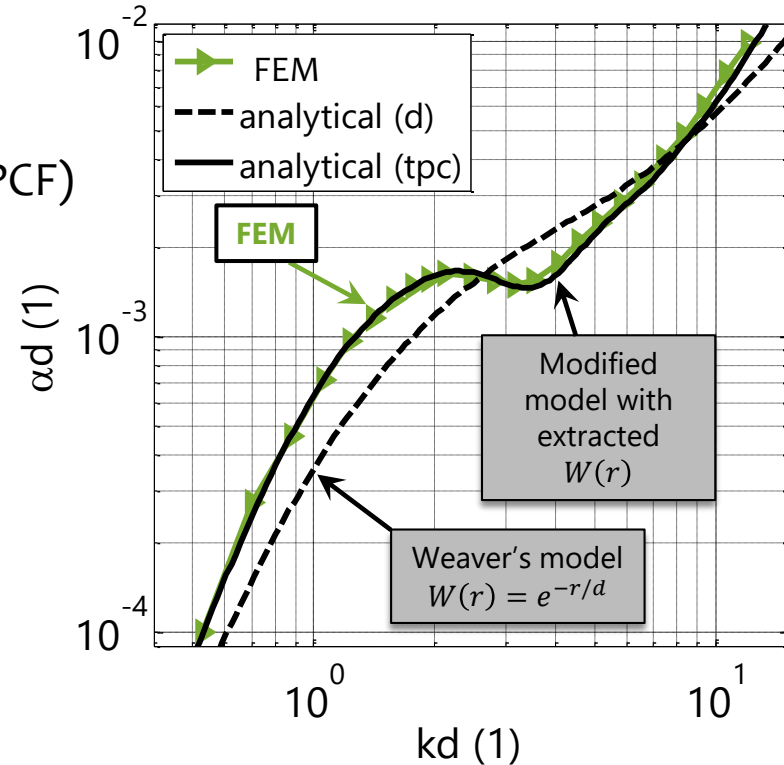
- Mean grain size d
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$$w(r) = e^{-r/d}$$

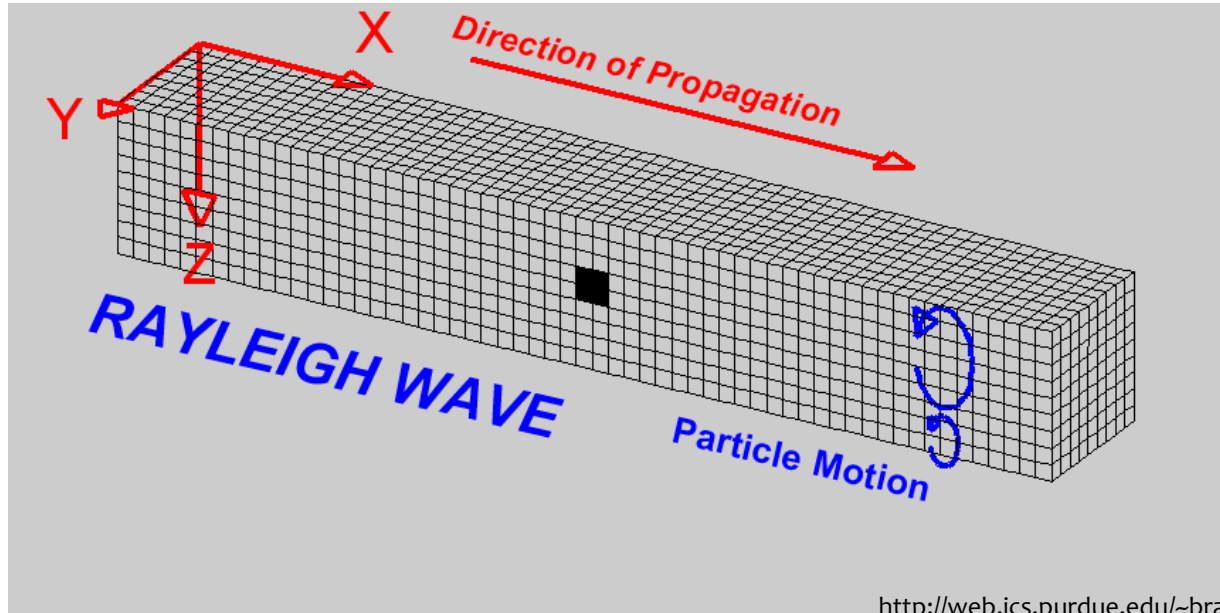
- Not in agreement with
the TPCF of the tessellation!

▣ Modified Weaver's model
with TPCF of the tessellation

TPCF as the crucial statistical parameter to describe the microstructure with respect to the scattering-induced attenuation!



- Grain-Boundary Scattering of Longitudinal Bulk waves
- **Grain-Boundary Scattering of Surface Acoustic Waves**

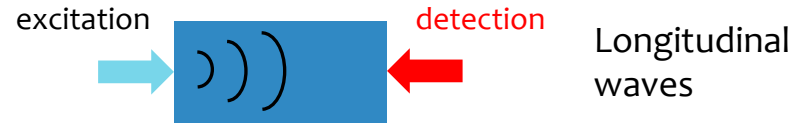
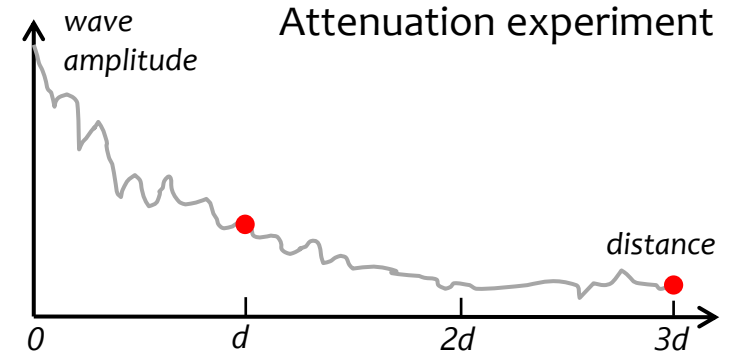


Why SAW?



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- Bulk-wave attenuation measurement at end points only

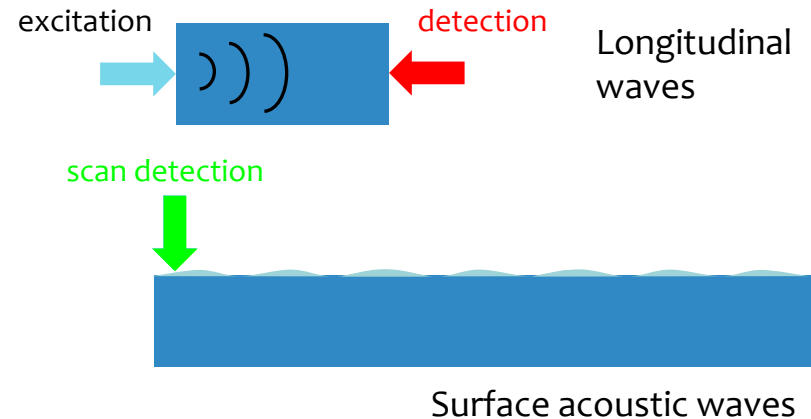
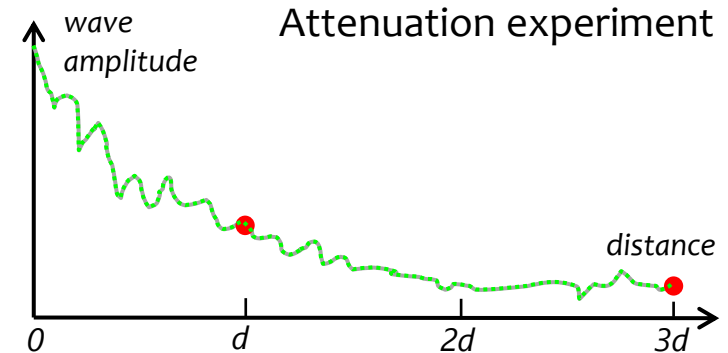


Why SAW?



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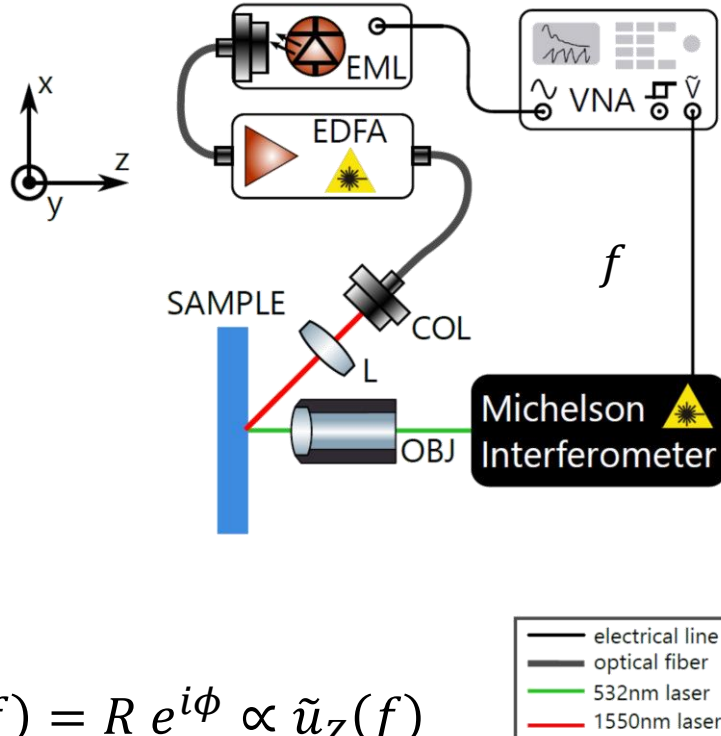
- Bulk-wave attenuation measurement at end points only
- SAW attenuation can be scanned!
 - ▣ Similar information as from simulation
 - ▣ Information from a near-surface layer
 - OK if homogeneous microstructure
 - ... Allows to study surface properties if not
 - Penetration depth depends on wavelength



Frequency-domain laser-ultrasonic setup



[M. Rzy et al., AIP Advances 8 (2018)]



$$\tilde{V}(f) = R e^{i\phi} \propto \tilde{u}_Z(f)$$

↓
Surface normal displacement

Excitation

- Electro-absorption modulated Laser diode (EML), $\lambda = 1.55\mu\text{m}$
→ $P=0.2\text{W}$
- Erbium doped fiber amplifier (EDFA)
→ $P \leq 1.2\text{W}$
- Point-source

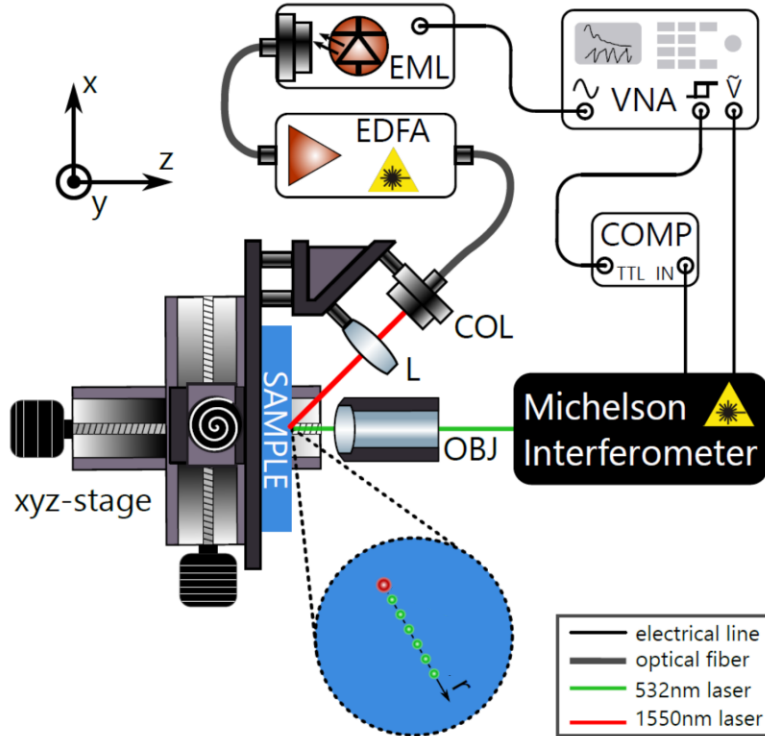
Detection

- Michelson interferometer
- Vector network analyzer (phase sensitive detection)
- Point-probe ($\lambda = 532\text{nm}$)

Frequency-domain laser-ultrasonic setup



[M. Rzy et al., AIP Advances 8 (2018)]



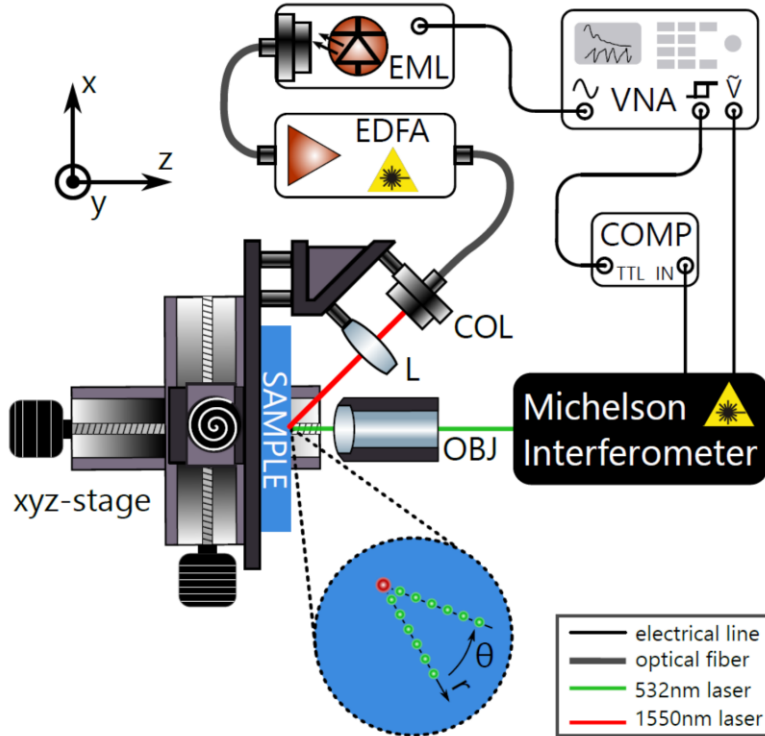
Get attenuation?

- Spatial scan
- Scan detection-point

Frequency-domain laser-ultrasonic setup



[M. Rzy et al., AIP Advances 8 (2018)]



Get attenuation?

- Spatial scan
- Scan detection-point

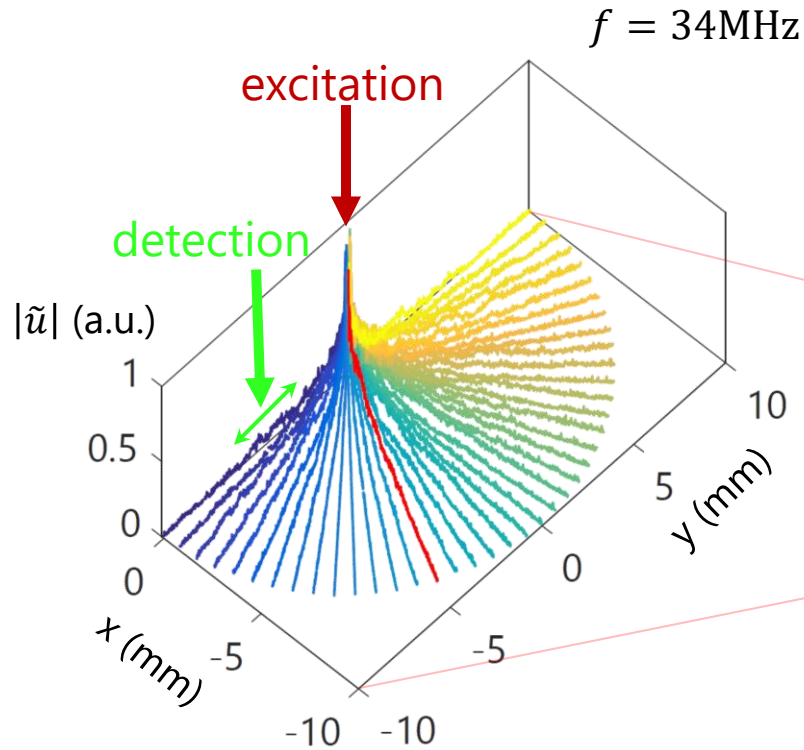
Get *averaged* attenuation?

- Spatial averaging
- Scan radial lines

Frequency-domain experiment

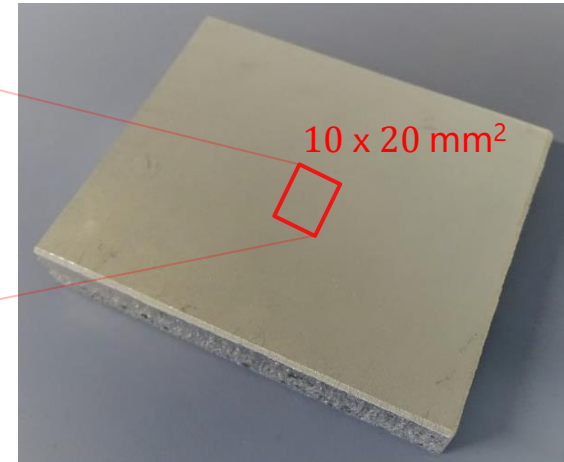


[M. Rzy et al., AIP Advances 8 (2018)]



Sample: Aluminum

$\approx 80 \times 80 \times 12 \text{ mm}^3$



mean grain size

$d \approx 94.5\mu\text{m}$

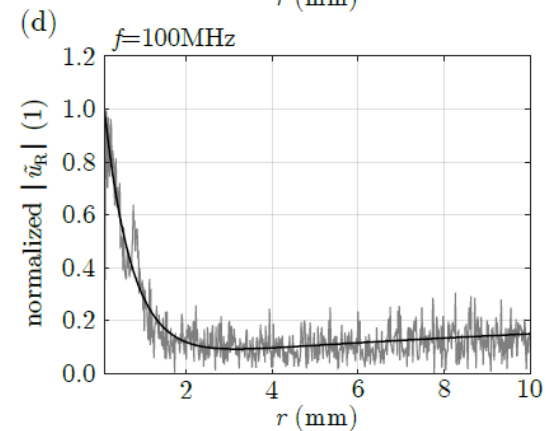
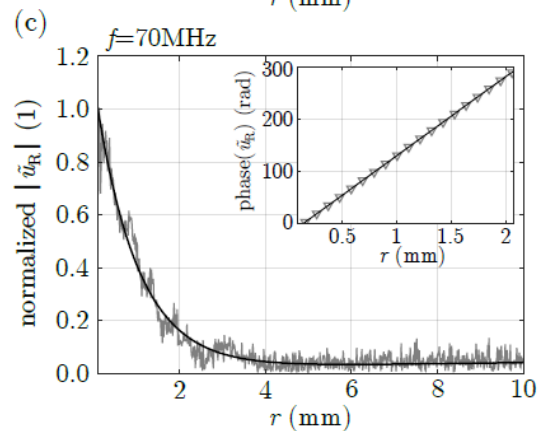
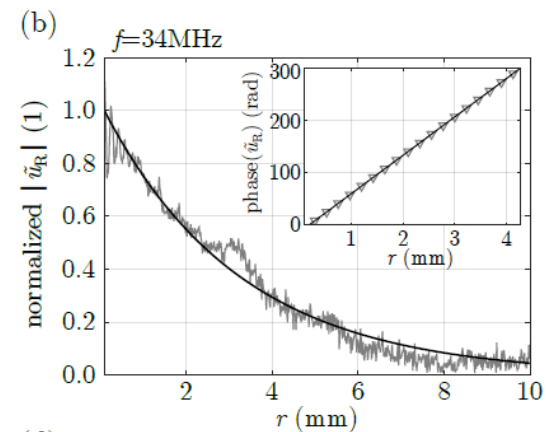
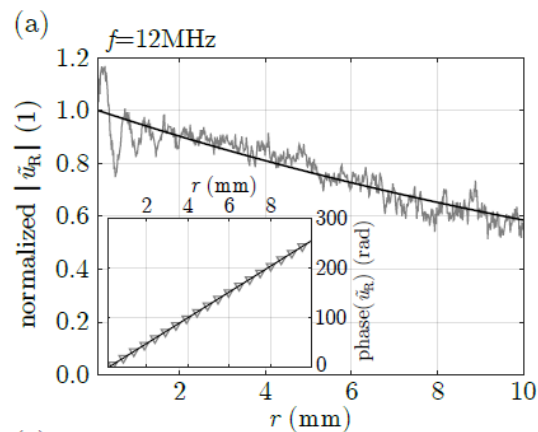
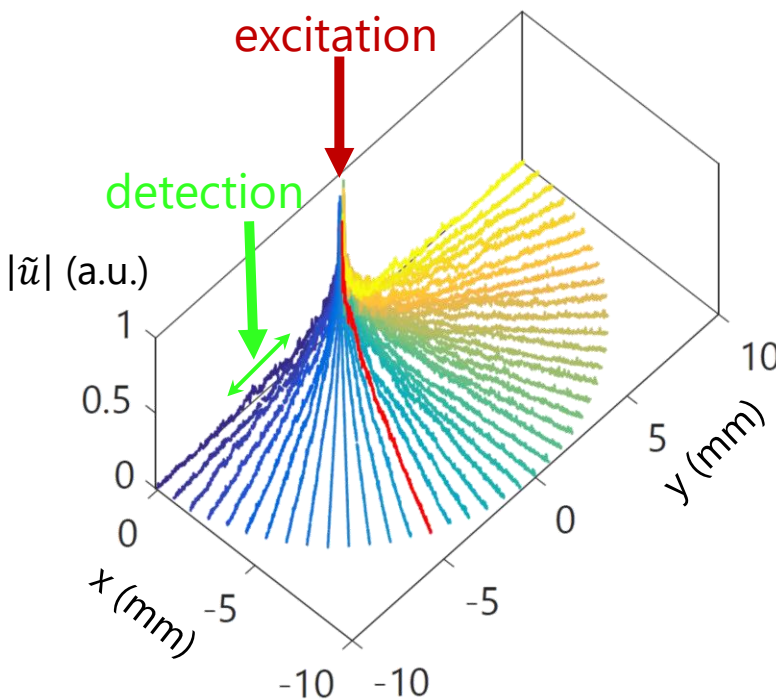
Frequency range: 10 ... 130MHz ($\Delta f = 2\text{MHz}$)

Spatial resolution: 15 μm

Frequency-domain attenuation



[M. Rzy et al., AIP Advances 8 (2018)]

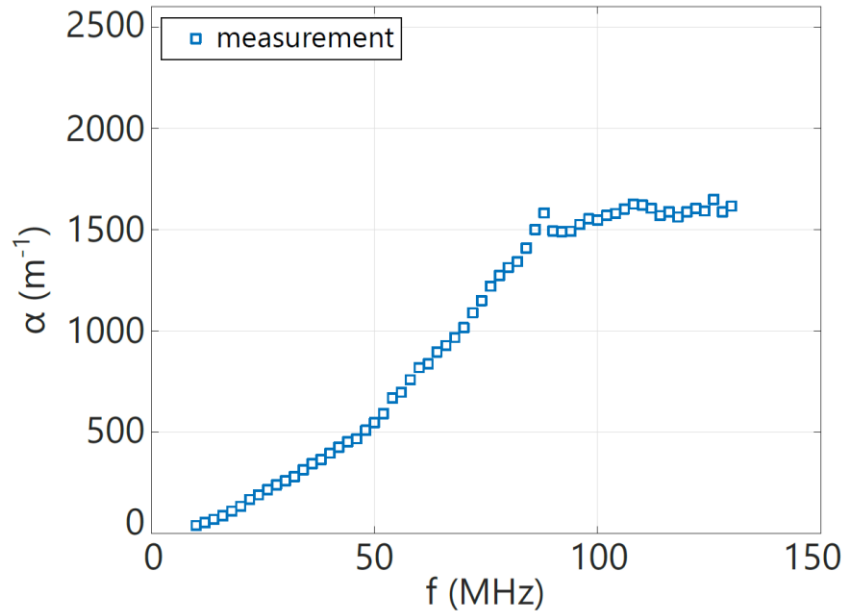


Experimental results



[M. Rzy et al., AIP Advances 8 (2018)]

Results (linear)



Two scattering-regimes?

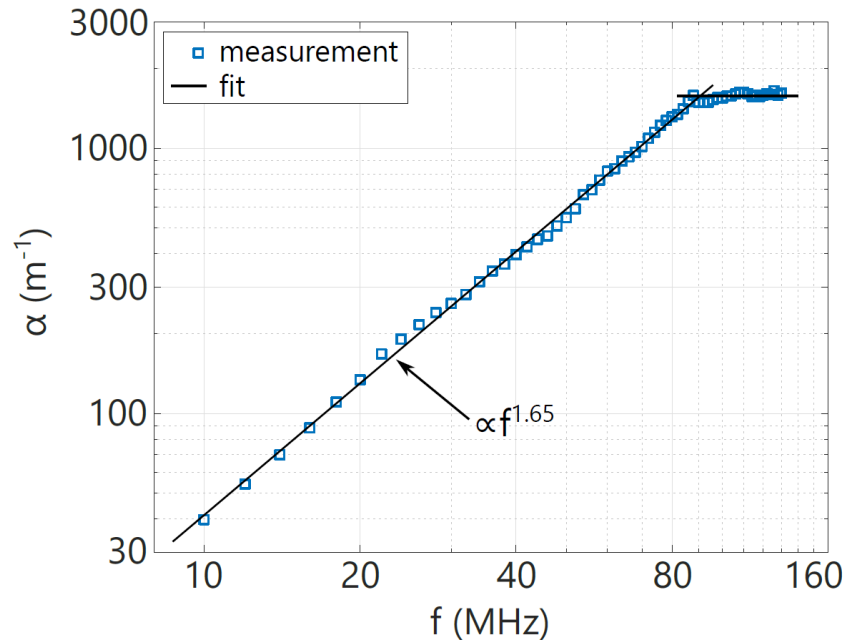
- Stochastic
 - Geometric
- ... but the higher frequencies already strongly attenuated

Experimental results



[M. Rzy et al., AIP Advances 8 (2018)]

Results (logarithmic)



$$c = (2892.8 \pm 4.0) \text{ms}^{-1}$$

Two scattering-regimes?

- \square Stochastic
- \square Geometric

... but the higher frequencies already strongly attenuated

Simple theoretical model for SAW



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[M. Rzy et al., AIP Advances 8 (2018)]

□ Assume that attenuation combined in a way similar to velocity

▣ Simple model:

- Modified Weaver's model
→ bulk-wave attenuation
- Rayleigh equation for surface wave in complex wavenumbers

Simple theoretical model for SAW



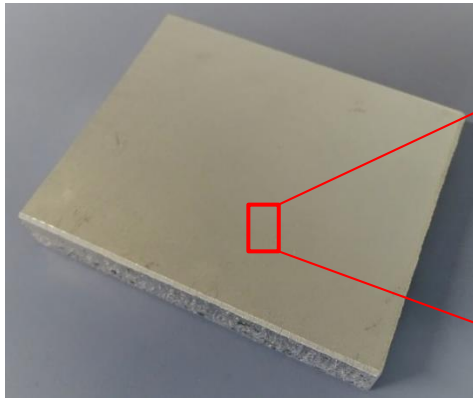
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[M. Rzy et al., AIP Advances 8 (2018)]

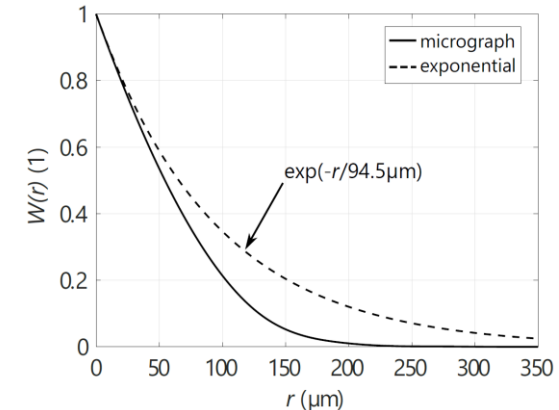
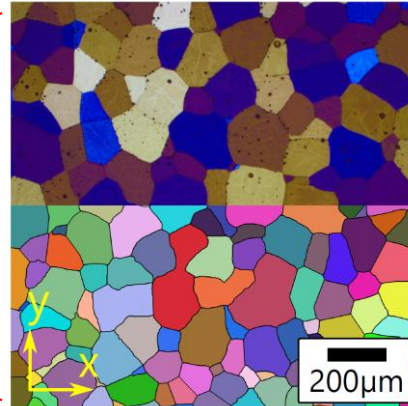
□ Assume that attenuation combined in a way similar to velocity

▣ Simple model:

- **Modified Weaver's model** → bulk-wave attenuation
 - **Rayleigh equation for surface wave** in complex wavenumbers
- TPCF of the sample necessary!



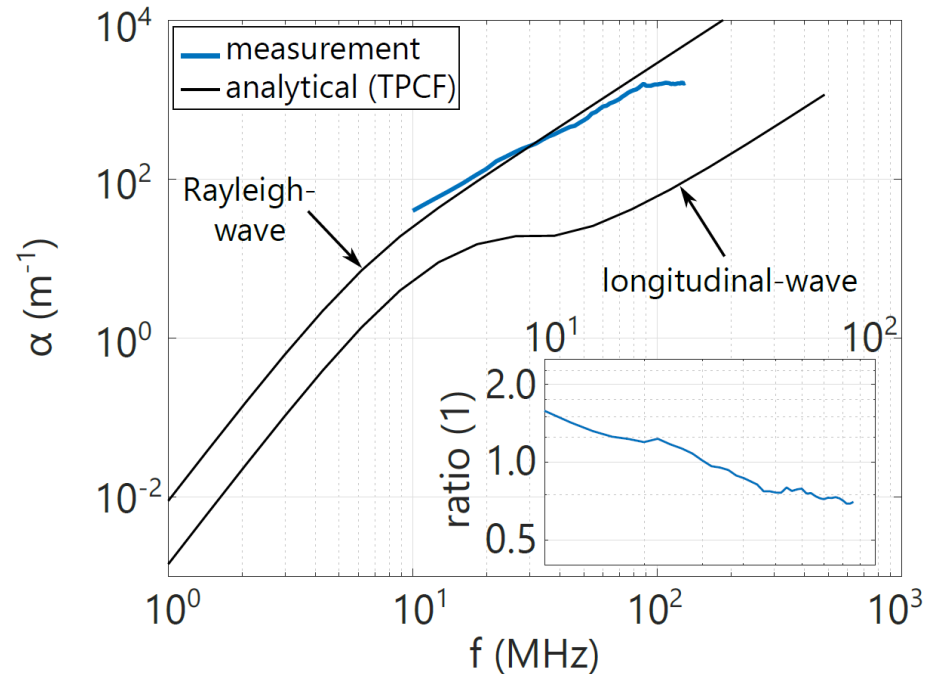
$\approx 80 \times 80 \times 12 \text{ mm}^3$



Experiment vs simple model



- Assume that attenuation combined in a way similar to velocity
 - ▣ Simple model:
 - Modified Weaver’s model
→ bulk-wave attenuation
 - Rayleigh equation for surface wave in complex wavenumbers
- Slightly different power-law dependence in stochastic regime (1.65 vs. 2.0)
- ▣ **Oversimplified analytical model or large experimental error?**



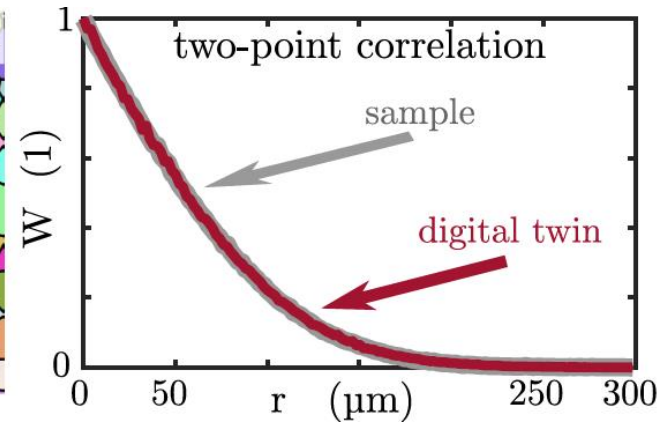
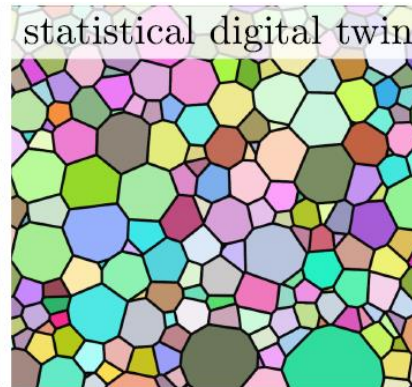
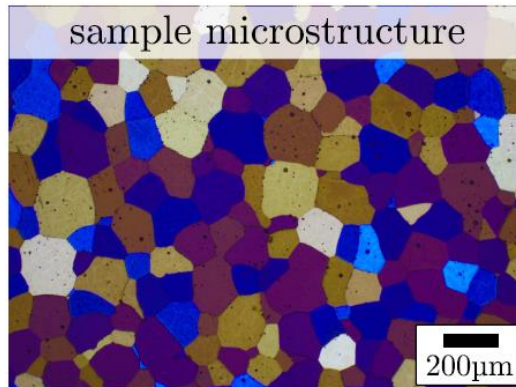
FEM simulation of SAW scattering



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[T. Grabec et al., Ultrasonics 119 (2022)]

- FEM simulation directly comparable to the experiment? (in a statistical way)
 - ▣ Model of the sample → Statistical digital twin (Laguerre tessellation)

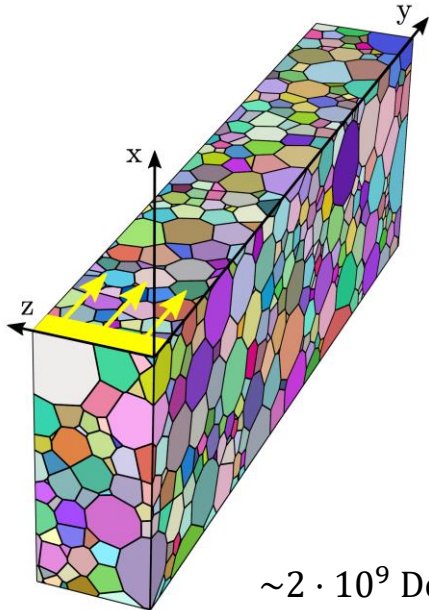


FEM simulation of SAW scattering

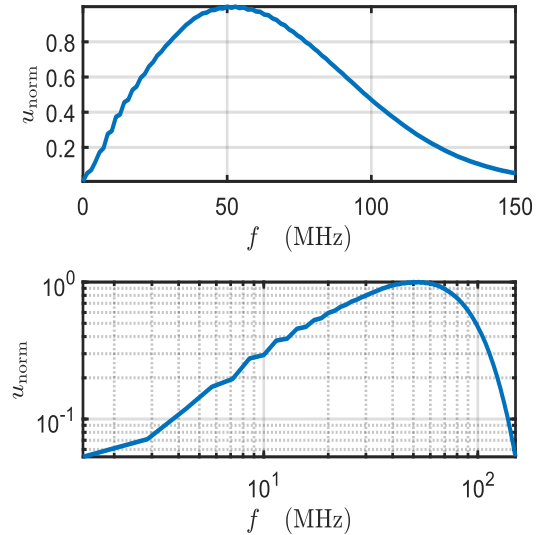


- FEM simulation directly comparable to the experiment? (in a statistical way)
 - ▣ Model of the sample → Statistical digital twin (Laguerre tessellation)
 - ▣ Broadband excitation:
 - Temporal and spatial gaussian profile

Frequency profile of SAW in homogeneous domain:



$\sim 2 \cdot 10^9$ DoF (60 runs)
elem . size $1.25 \mu\text{m}$, time step 0.9 ns



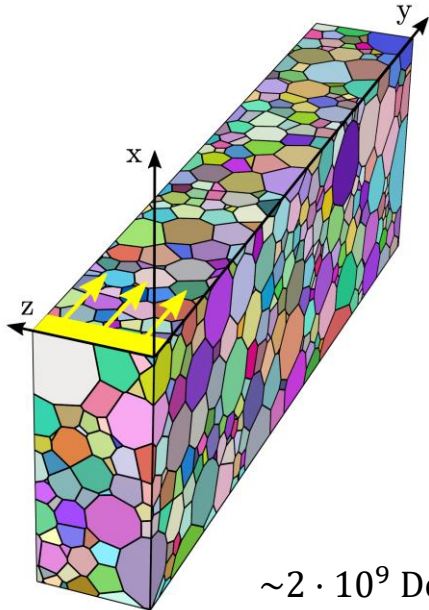
FEM simulation of SAW scattering



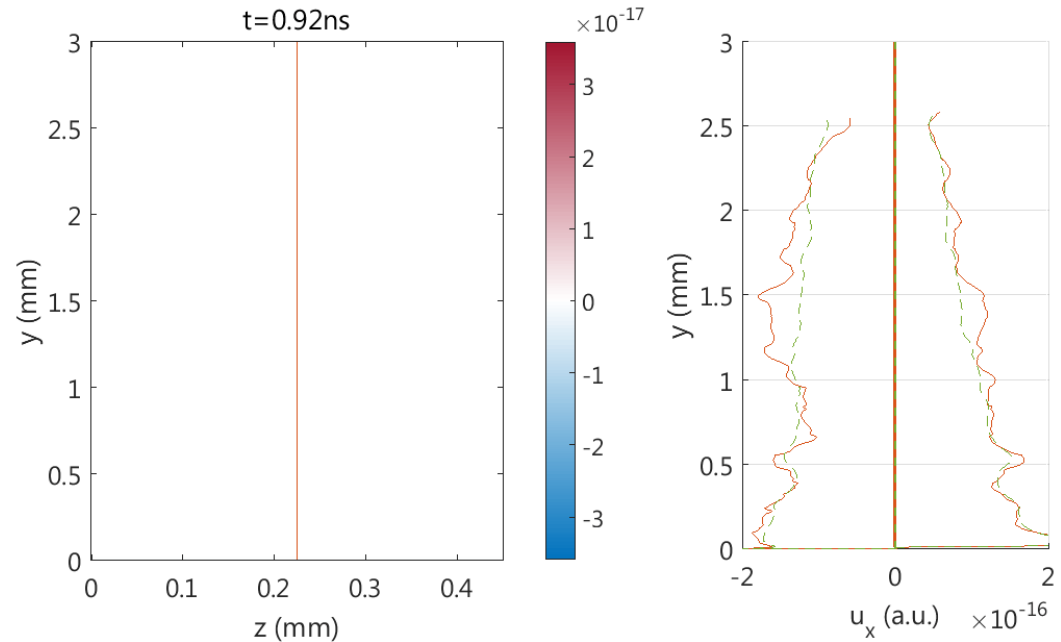
27

[T. Grabec et al., Ultrasonics 119 (2022)]

- FEM simulation directly comparable to the experiment? (in a statistical way)
 - Model of the sample → Statistical digital twin (Laguerre tessellation)
 - Broadband excitation → gaussian



$\sim 2 \cdot 10^9$ DoF (60 runs)
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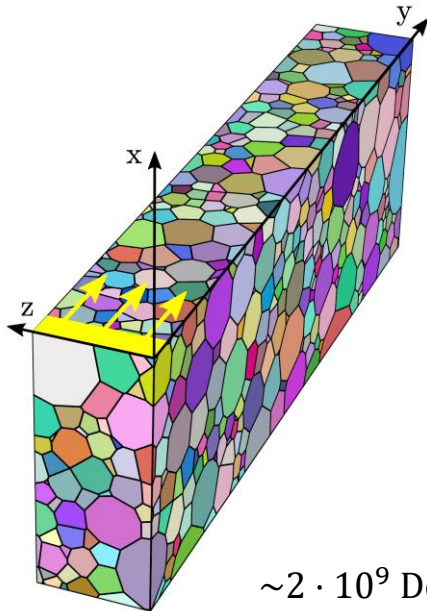
FEM simulation of SAW scattering



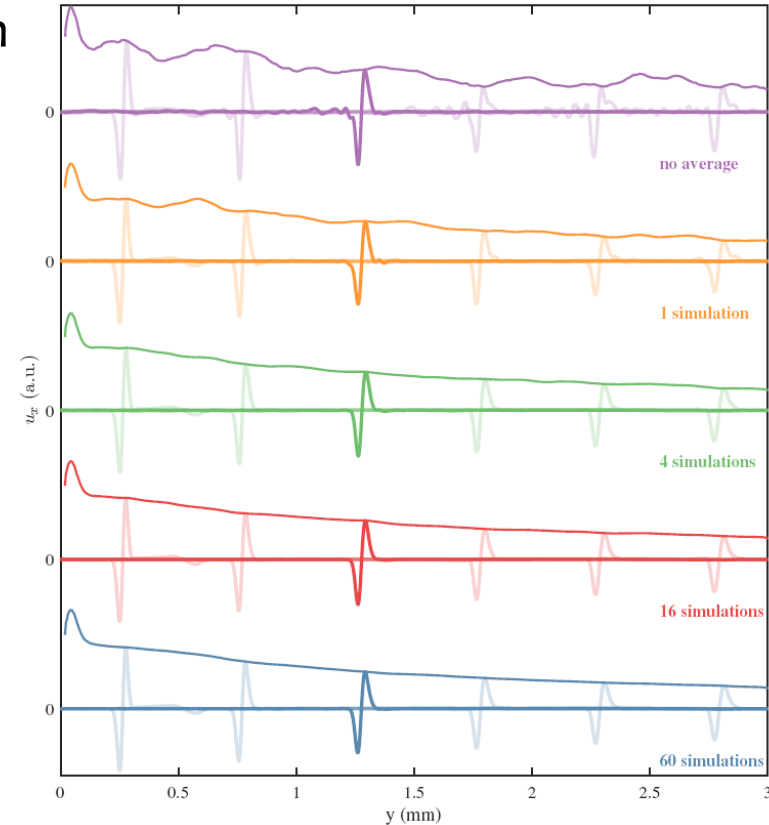
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[T. Grabec et al., Ultrasonics 119 (2022)]

- FEM simulation directly comparable to the experiment? (in a statistical way)
 - Model of the sample → Statistical digital twin
 - Broadband excitation → gaussian
 - Large number of repetitive runs to obtain the averaged response



$\sim 2 \cdot 10^9$ DoF (60 runs)
elem . size $1.25 \mu\text{m}$, time step 0.9 ns



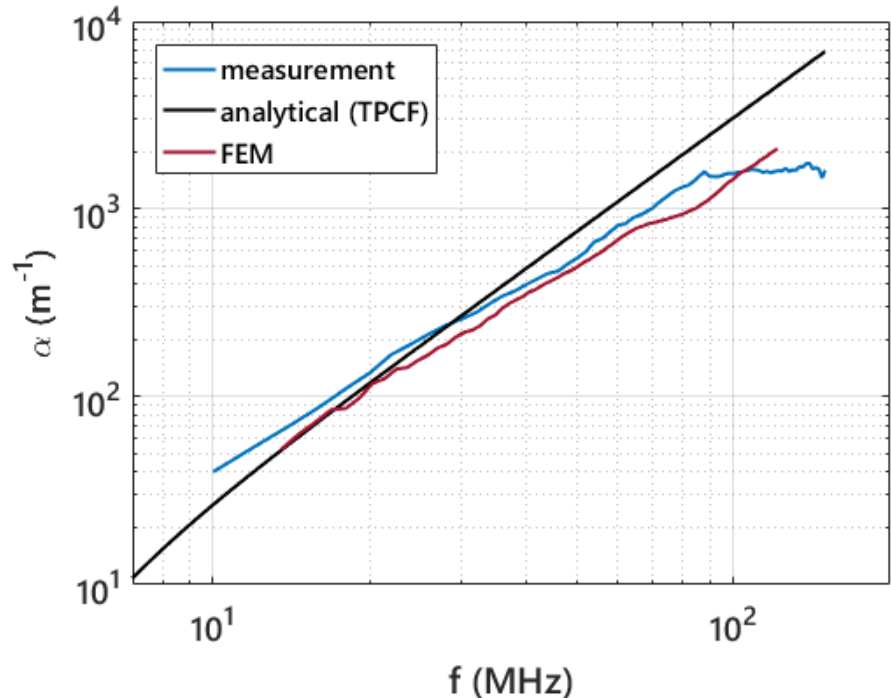
Simulation vs Experiment vs Model



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[T. Grabec et al., Ultrasonics 119 (2022)]

- Simulation in great agreement with the experiment!
→ better than with the model
- Both experiment and FEM suggest different slope (power-law exponent) than for bulk waves
→ more complex analytical description necessary!
- Apparent geometric region in experiment not shown by FEM
→ probably a result of large error in experiment at higher frequencies



Conclusion

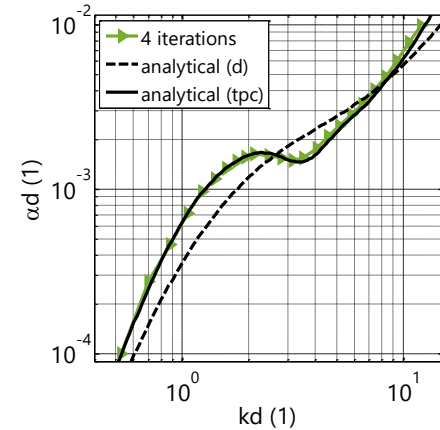
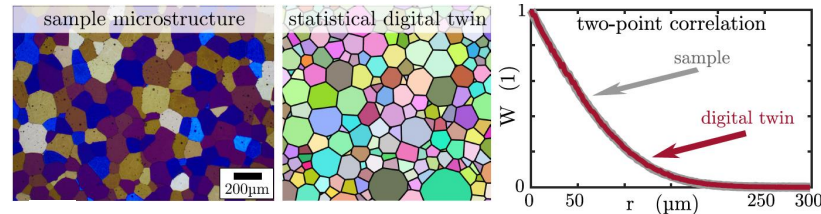


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Analysis of L-wave attenuation:

- Importance of two-point correlation function (TPCF) for microstructure description:

Excellent fit of TPCF-corrected analytical model with FEM simulation



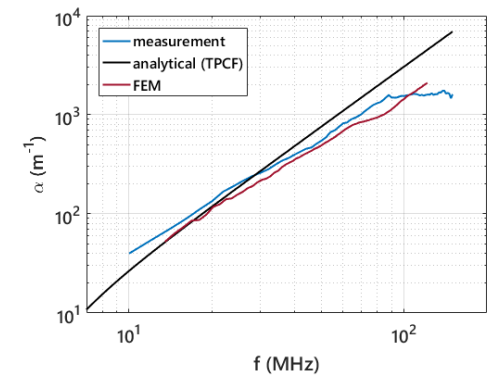
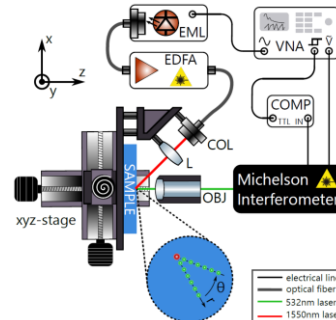
SAW attenuation:

- Simple model proposed – combining Weaver’s model with Rayleigh equation in complex wavenumbers

- Frequency-dependent attenuation measured experimentally using laser-ultrasonic setup

- FEM simulations on sample-mimicking tessellation

- Excellent agreement between simulation and experiment



Conclusion

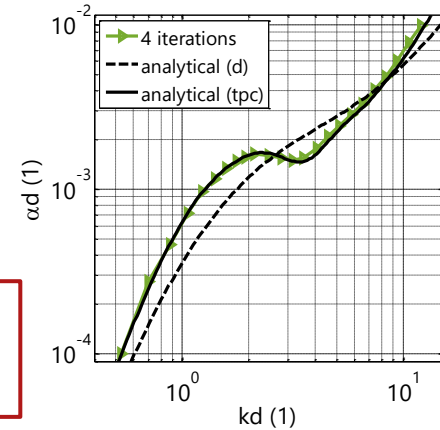


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Analysis of L-wave attenuation:

- Importance of two-point correlation function (TPCF) for microstructure description:

Excellent fit of TPCF-corrected analytical model with FEM simulation



Thank you for attention!

SAW att

- Simple model proposed
 - combining Weaver’s model with Rayleigh equation in complex wavenumbers
- Frequency-dependent attenuation measured experimentally using laser-ultrasonic setup
- FEM simulations on sample-mimicking tessellation
- Excellent agreement between simulation and experiment

