Grain-boundary Scattering of Surface Acoustic Waves: Experiment, Theory, and Simulation

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Outline

- Grain-Boundary Scattering of Longitudinal Bulk Waves
- Grain-Boundary Scattering of Surface Acoustic Waves
FEM simulation of L-wave scattering

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

8000 grains
1 × 2 × 2 mm³

375 mil. DoF (12 runs)
el. size 3.2 μm, time step 0.4 ns

Tessellation Software: Neper
FEM Software: PzFlex

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Time-domain FEM simulation of longitudinal-wave propagation

Coherent wave and attenuation

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

ballistic wave
Coherent wave and attenuation

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

Attenuation
- Macroscopic
- Effective medium

‘coherent wave’
Coherent wave and attenuation

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

Coherent wave
\[ \langle \tilde{u} \rangle(x, \omega) \propto e^{i(\mathbf{k}x - \omega t)} \]
\[ \frac{\omega}{c(\omega)} + i \alpha(\omega) \]

Effective homogeneous medium with only parametrical description of the microstructure

Attenuation
- Macroscopic
- Effective medium

'coherent wave'
Scattering Regimes & Asymptotes

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

  Analytical (attenuation) model

  e.g.: Weaver’s model  

\[
\begin{align*}
\lambda &\ll d & \alpha &\propto \frac{1}{d} \\
\lambda &\gg d & \alpha &\propto d^3 f^4 \\
\lambda &\approx d & \alpha &\propto d f^2 \\
\end{align*}
\]
Simulation vs Experiment

- Weak agreement with the model
  - Microstructure description?
    - Mean grain size $d$
    - and assumed two-point correlation function (TPCF)
    \[ w(r) = e^{-r/d} \]

[Weaver's model, FEM]

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

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- 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!
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L. Braile, Purdue University
http://web.ics.purdue.edu/~braile/edumod/waves/WaveDemo.htm
Why SAW?

- Bulk-wave attenuation measurement at end points only
Why SAW?

- 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
Excitation

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

Detection

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

\[ \tilde{V}(f) = Re^{i\phi} \propto \tilde{u}_Z(f) \]

Surface normal displacement

[M. Ryzy et al., AIP Advances 8 (2018)]
Frequency-domain laser-ultrasonic setup

Get attenuation?
- Spatial scan
- Scan detection-point

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Get *averaged* attenuation?
- Spatial averaging
- Scan radial lines
Frequency-domain experiment

Frequency range: 10 ... 130MHz ($\Delta f = 2$MHz)
Spatial resolution: 15µm

Sample: Aluminum

$\approx 80 \times 80 \times 12$ mm$^3$

$10 \times 20$ mm$^2$

mean grain size

$d \approx 94.5$µm
Frequency-domain attenuation

|\tilde{u}| (a.u.)

excitation
detection

[M. Ryzy et al., AIP Advances 8 (2018)]
Experimental results

Two scattering-regimes?
- Stochastic
- Geometric

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

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

[M. Ryzy et al., AIP Advances 8 (2018)]
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- **Modified Weaver’s model** → bulk-wave attenuation
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TPCF of the sample necessary!

\[ \approx 80 \times 80 \times 12 \text{ mm}^3 \]
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?**

[M. Ryzy et al., AIP Advances 8 (2018)]
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)
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- 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 μm, time step 0.9 ns

[T. Grabec et al., Ultrasonics 119 (2022)]
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FEM simulation of SAW scattering

- 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)
elen . size 1.25 $\mu$m, time step 0.9 ns

[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**

- **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
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Thank you for attention!