Simulation of ultrasound propagation in anisotropic polycrystalline media

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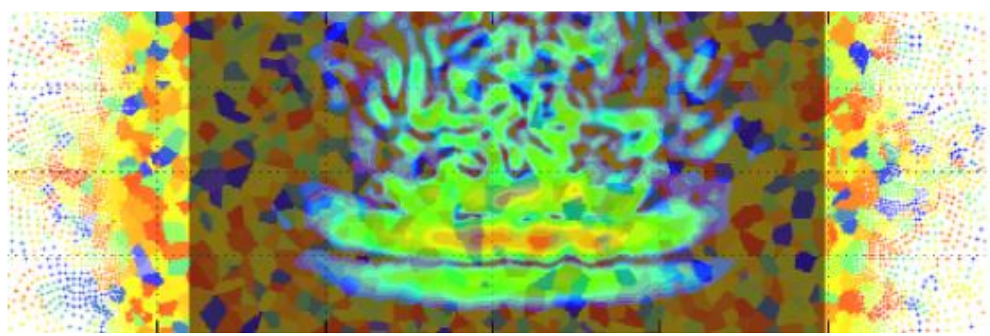


Motivations

- ✓ Construct a simulation tool to examine the ultrasound properties in a sample with:
  - ✓ A given geometry
  - ✓ A particular crystallographic structure (stiffness)
  - ✓ A certain crystallographic arrangement (texture)
  - ✓ A controlled grain size distribution
  - ✓ A second phase, grain morphology, …
- ✓ Examine the relative change of a particular ultrasound parameter as one of the above evolves

What do we need ?

- Three main requisites
  - Materials properties (stiffness, density, grain size, morphology and crystallographic orientation)
  - Finite Element engine (Sample geometry, meshing, wave generation, propagation and detection of pulse)
  - Waveform analysing tool (Extract ultrasound pulse properties, velocities, attenuation spectrum)

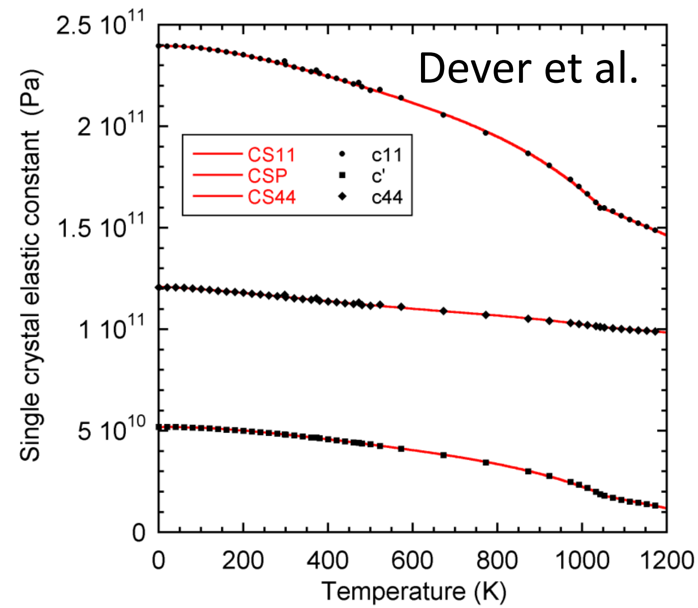
Materials properties

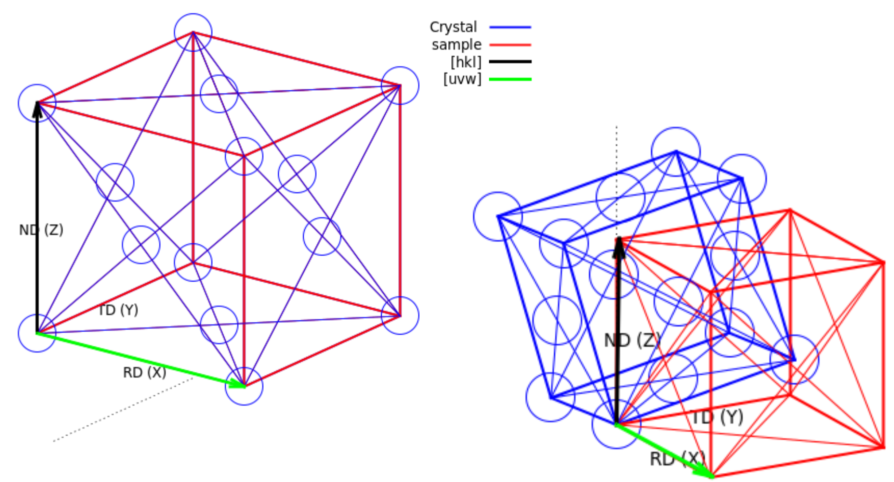
✓ BCC-iron (well documented, relatively highly anisotropic)

$$\boldsymbol{\sigma} = \boldsymbol{c} : \boldsymbol{\epsilon}$$

✓ Rotation of stiffness tensor (Euler’s angles)

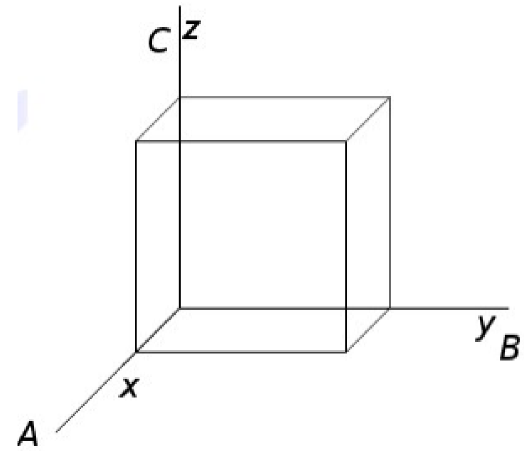
$$\boldsymbol{c}' = \boldsymbol{M}_{ZYZ}\, \boldsymbol{c}\, \bar{\boldsymbol{M}}_{ZYZ}$$





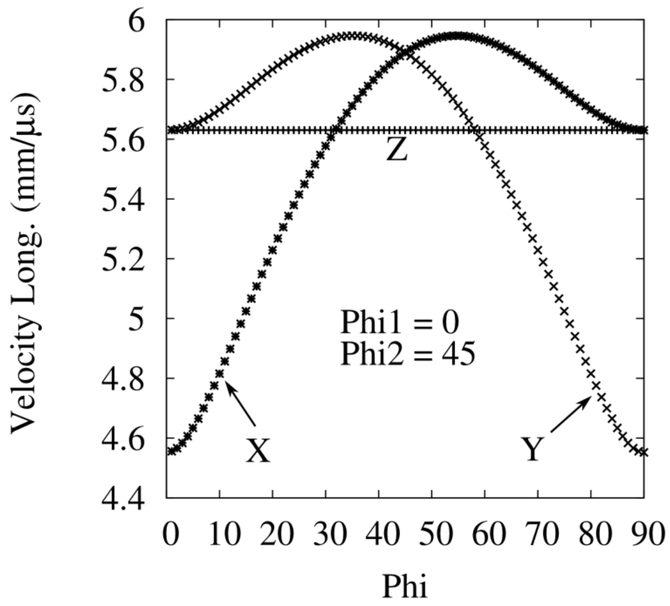
Crystal orientation, propagation direction

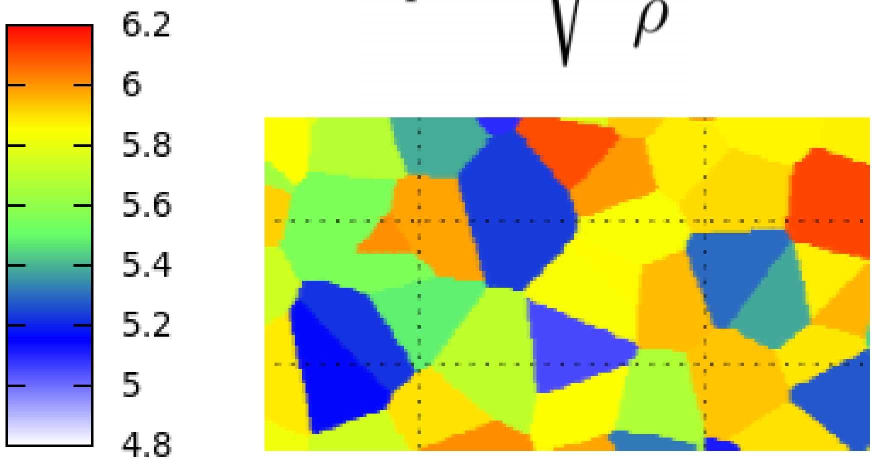
- ✓ Wave propagating in a particular direction of the sample



$$T_{ik}(\vec{n}) = C_{ijkl}\vec{n}_j\vec{n}_l$$

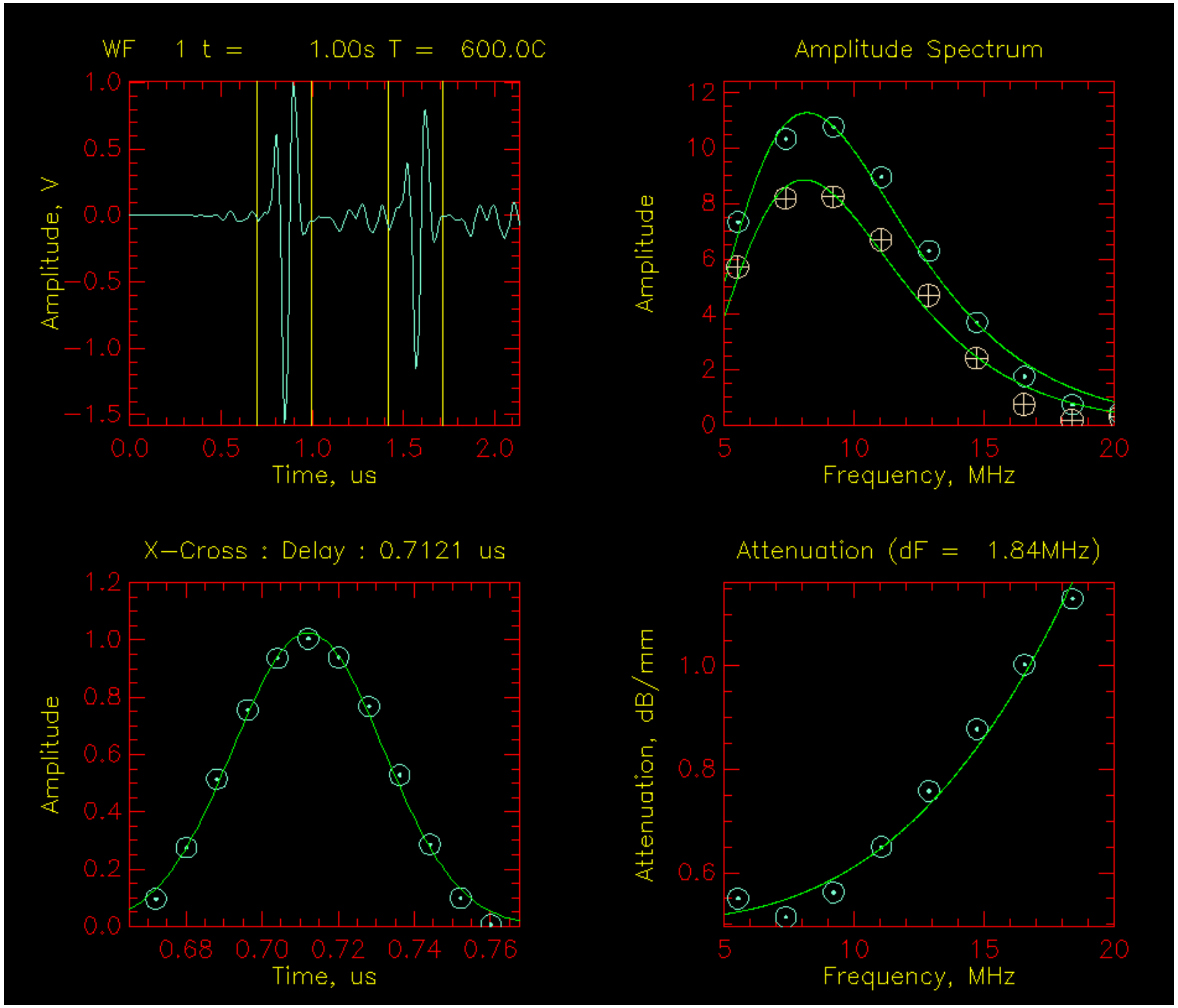
$$V_p = \sqrt{\frac{\lambda_1}{\rho}}$$





Waveform analysis

- ✓ Fortran software
- ✓ Windowing, Cross-correlation, spectrum evaluation
- ✓ Velocity, attenuation

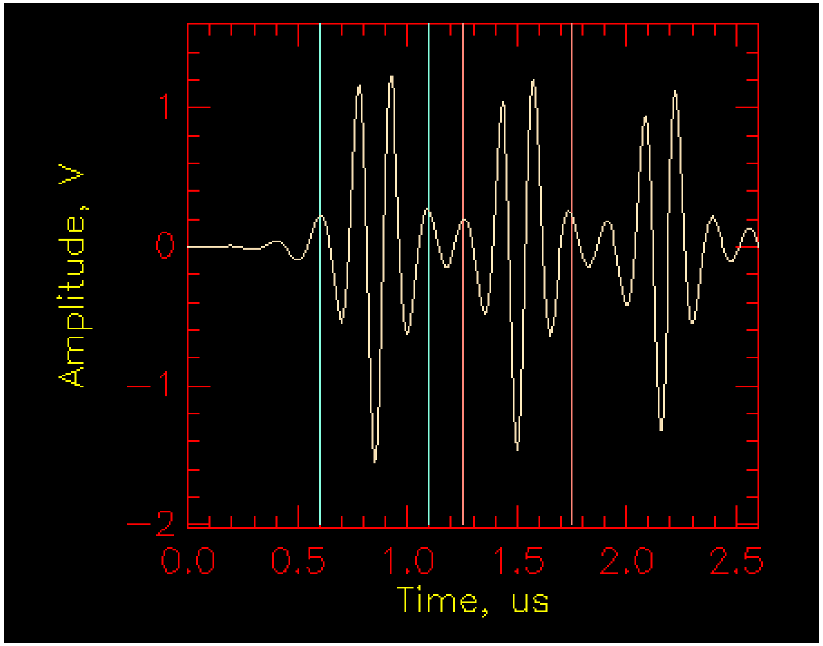


Generation pulse

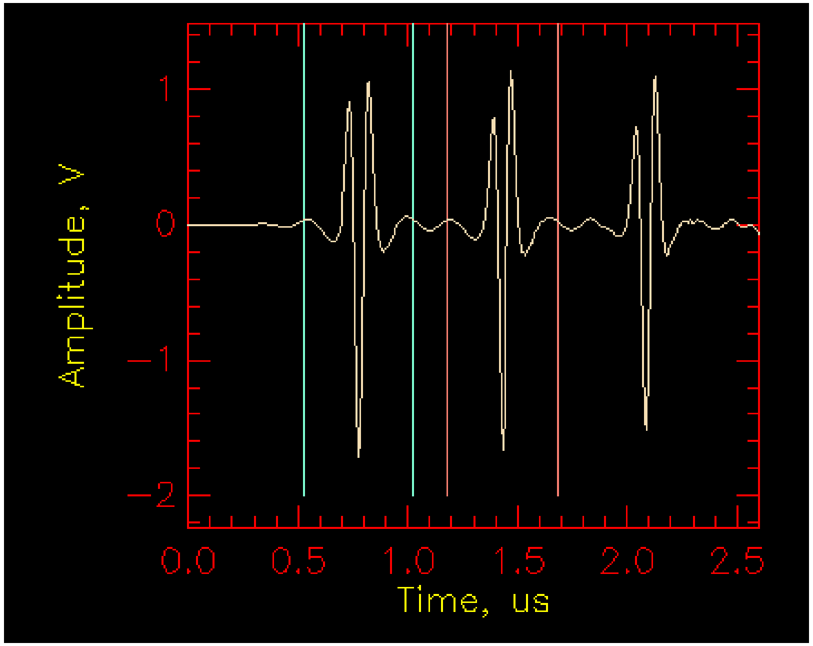
✓ Ricker wavelet, fine tune of the center frequency and bandwidth available

$$A = (1 - 2\pi^2 f^2 t^2) e^{-\pi^2 f^2 t^2}$$

7MHz



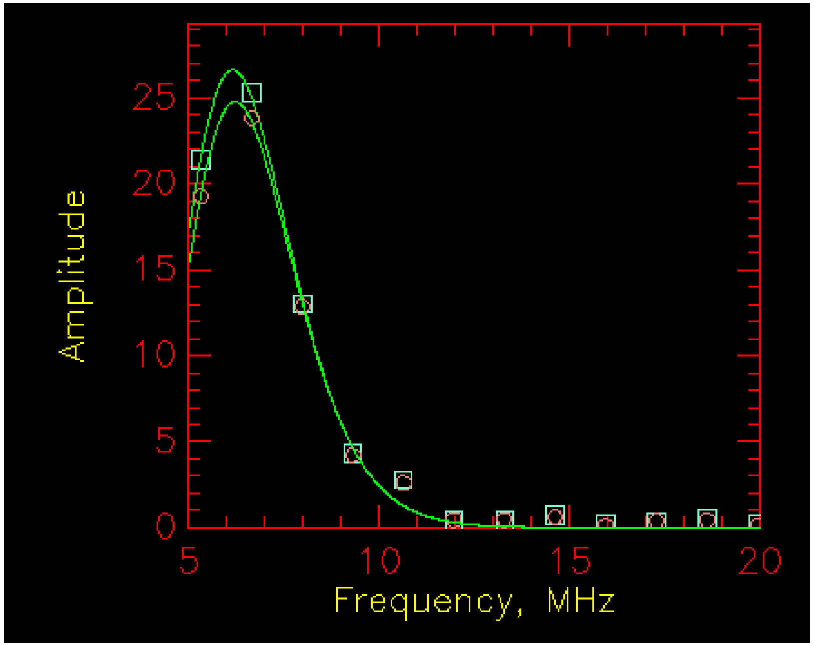
10MHz



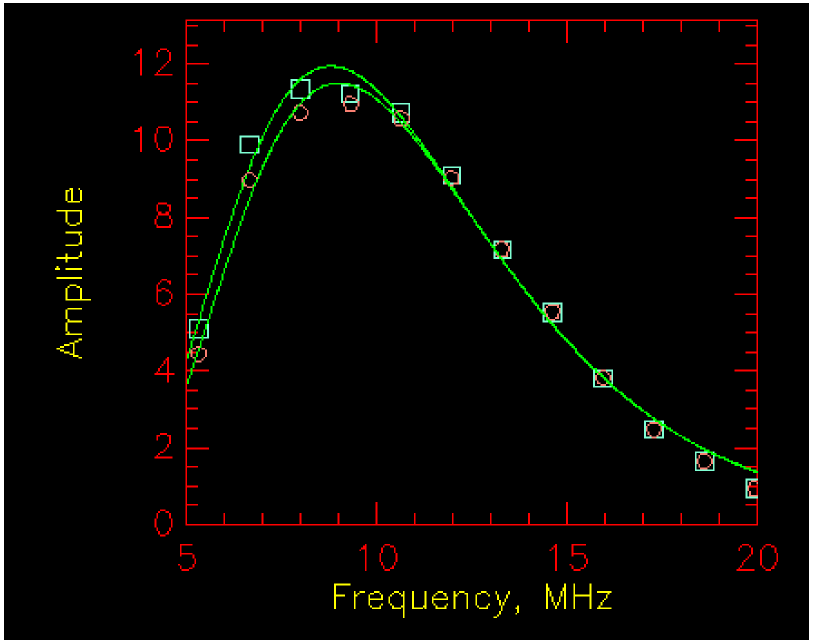
Bandwidth, frequency resolution

- ✓ Frequency resolution relates to the windows size
- ✓ Bandwidth relates to the center frequency

7MHz

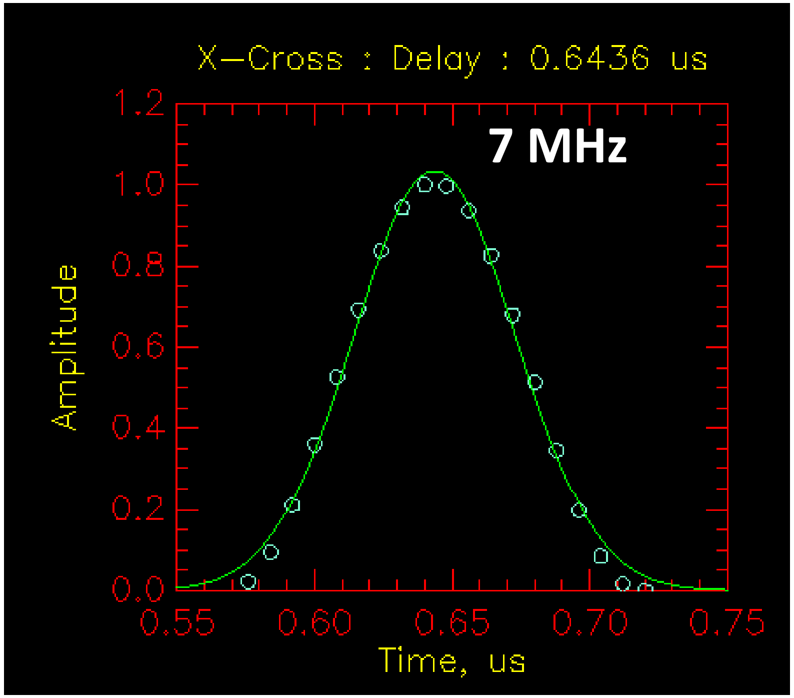


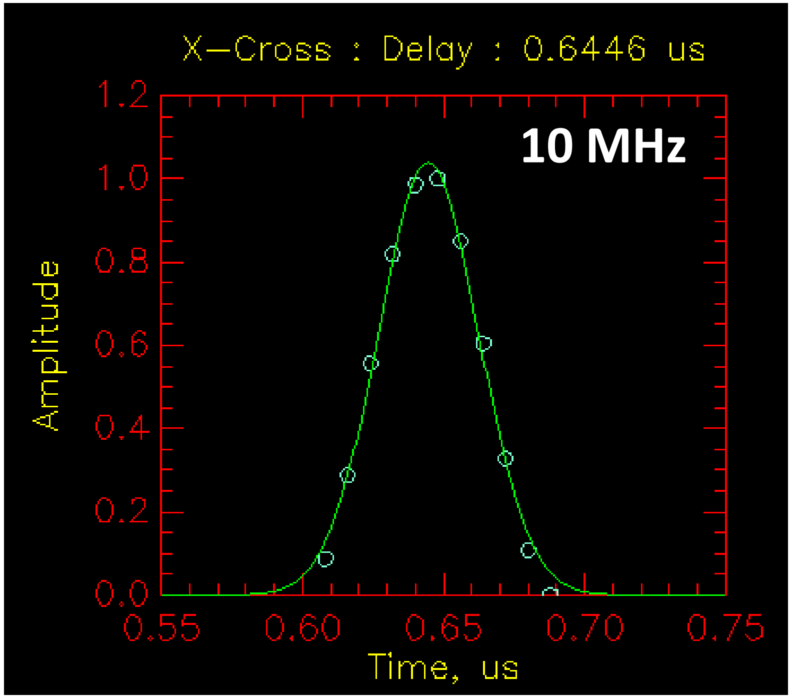
10MHz



Time resolution for delay

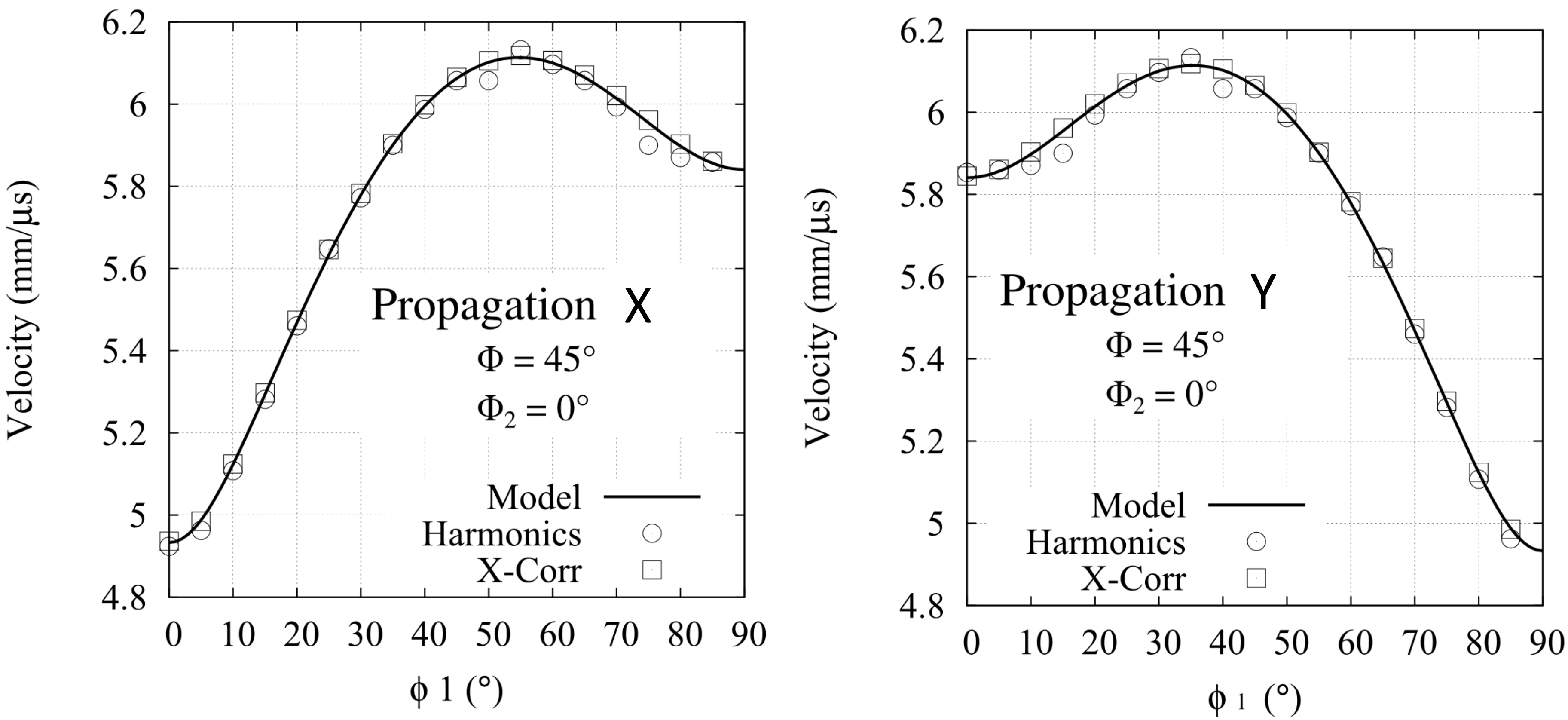
- ✓ Gaussian interpolation of the maximum of a cross-correlation function between two echoes
- ✓ Accuracy 1 ns, equivalent to a relative change in the bulk modulus of 1GPa





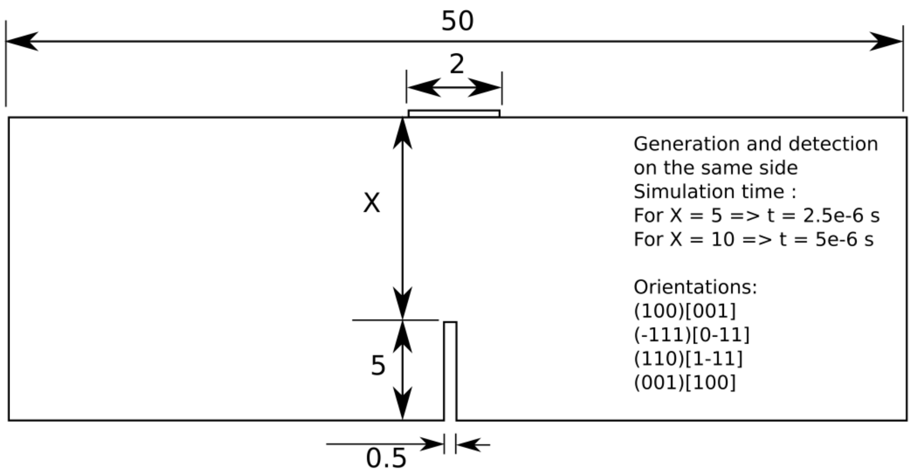
Ultrasound velocity in single crystal

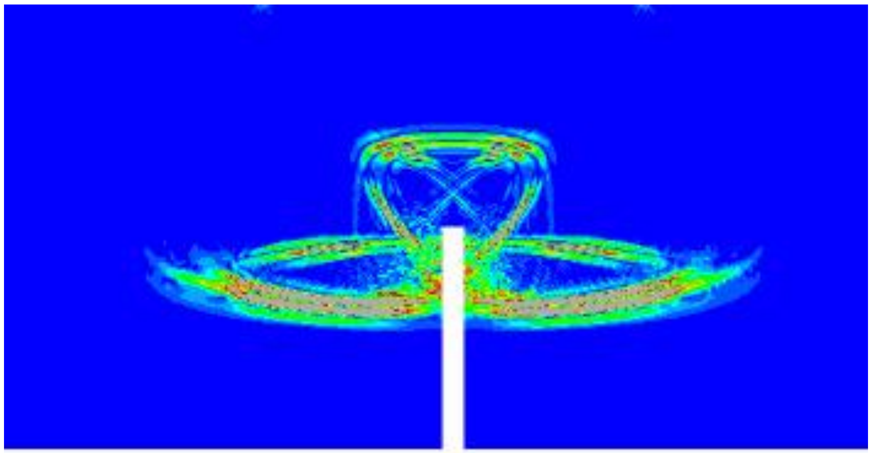
✓ Wave propagating along the X, Y in single crystal with specific crystallographic orientation



Ultrasound dispersion in single crystal

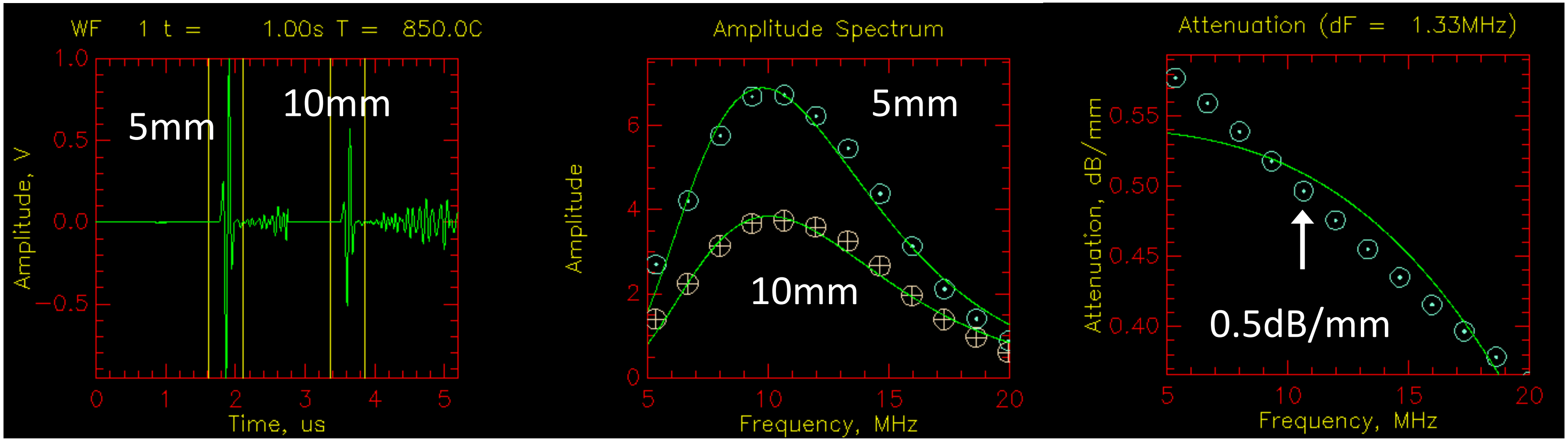
- ✓ Wave propagating in single crystal with specific crystallographic orientation
- ✓ Evaluation of the dispersion of the ultrasound pulse with respect to the crystallographic orientation



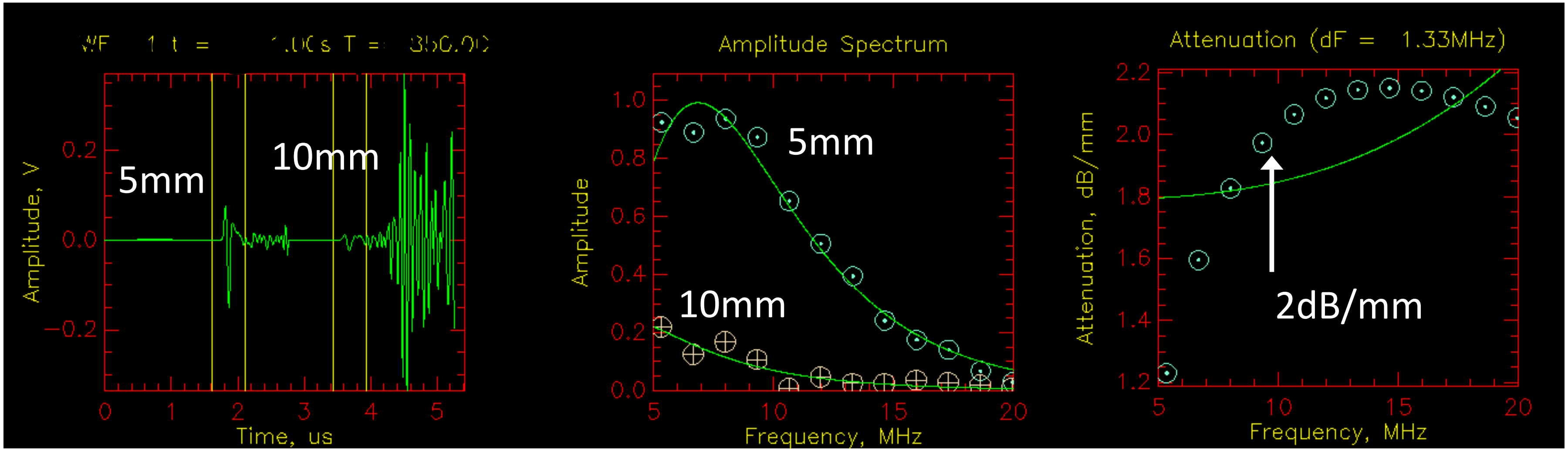


Ultrasound dispersion in single crystal

✓ Orientation (1 0 0) [0 0 1] : Weak dispersion

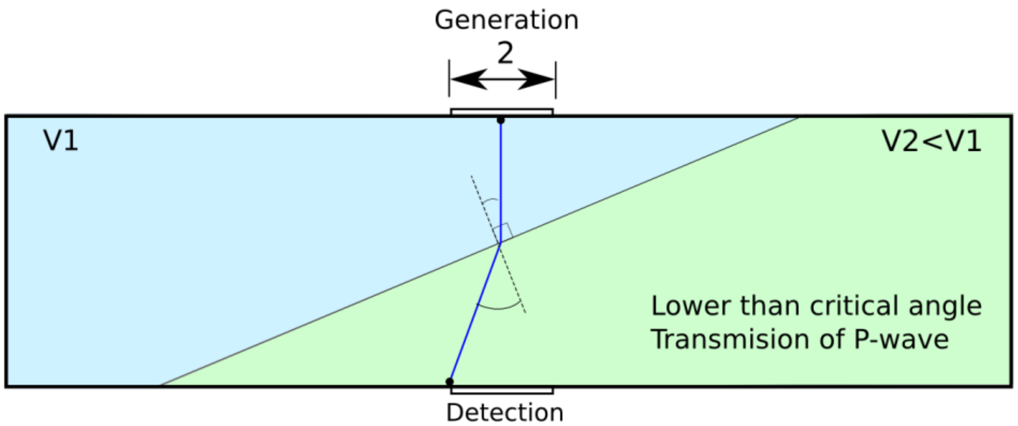


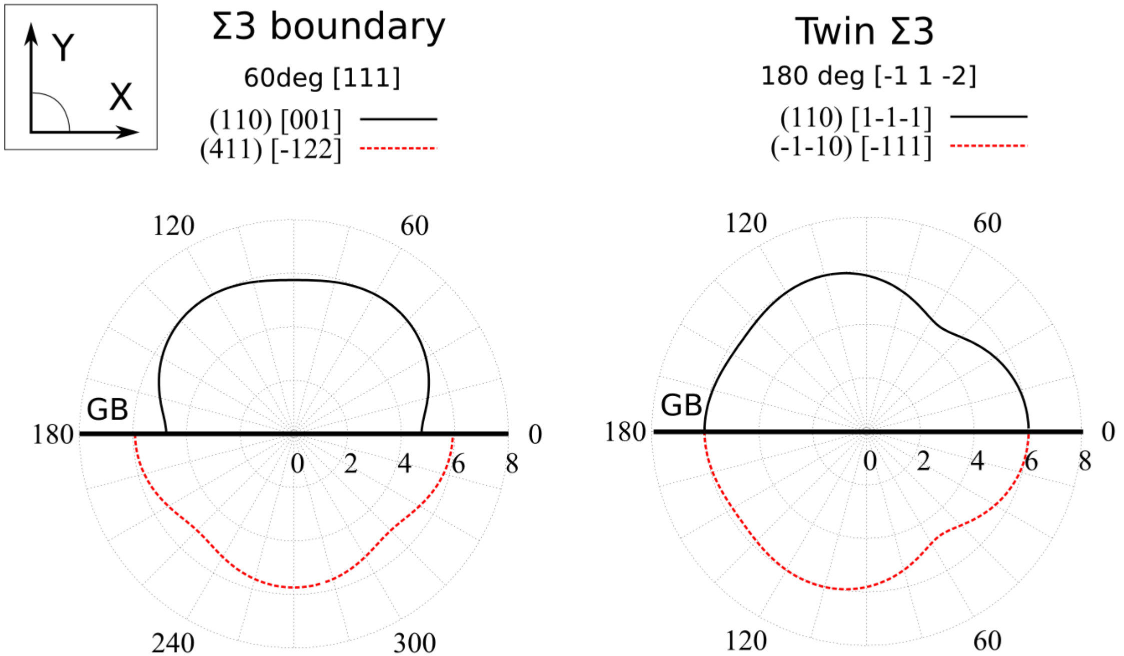
✓ Orientation (1 1 0) [1 -1 1] : Strong dispersion



Bi-crystal: misorientation, incidence angle

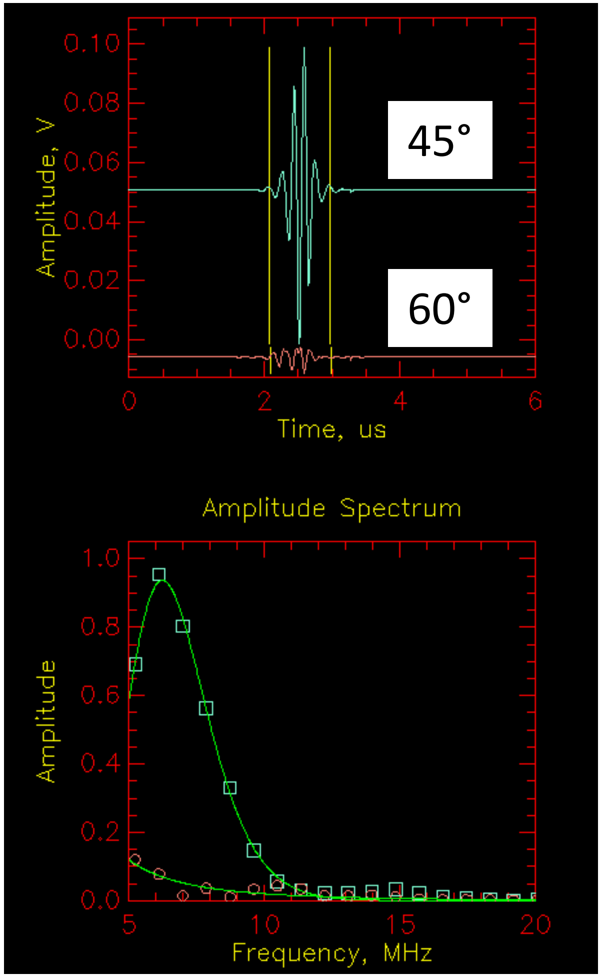
- ✓ Study of incidence angle with grain boundary
- ✓ Effect of misorientation between two grains
- ✓ Anisotropic elastic mismatch between two grains

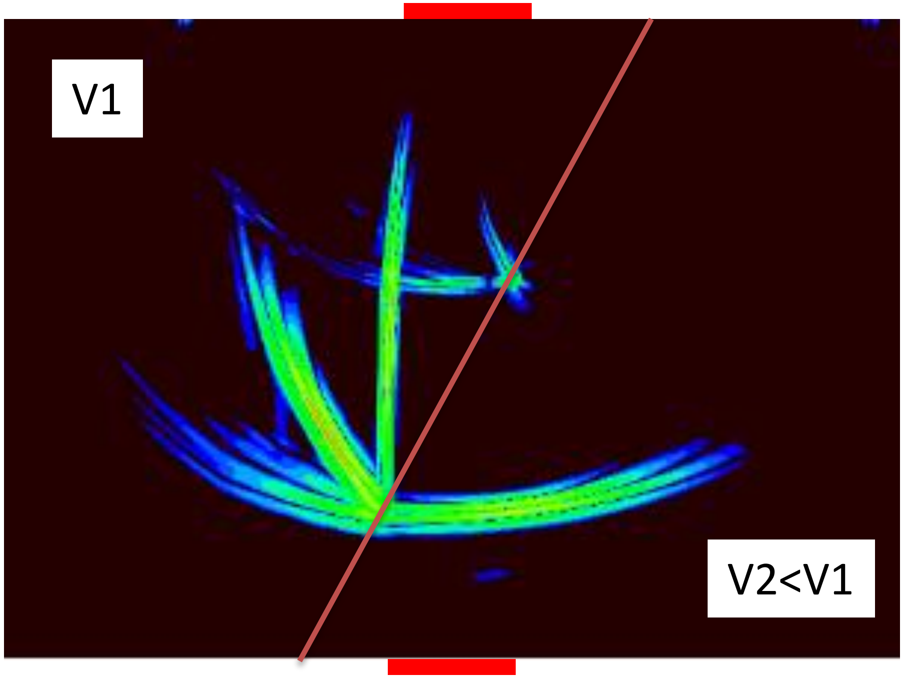




Bi-crystal: isotropic case

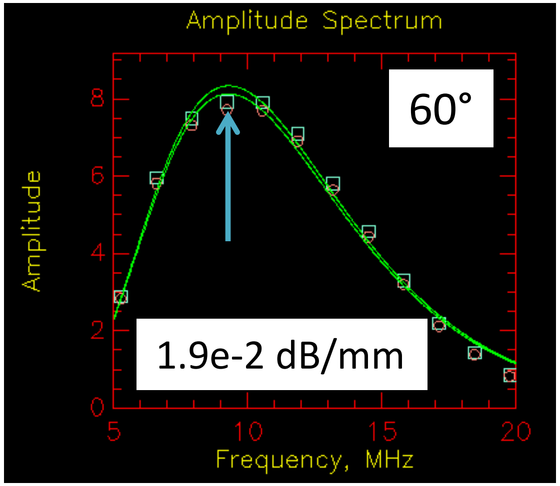
- ✓ Compare energy collected at 45° with higher incidence angle

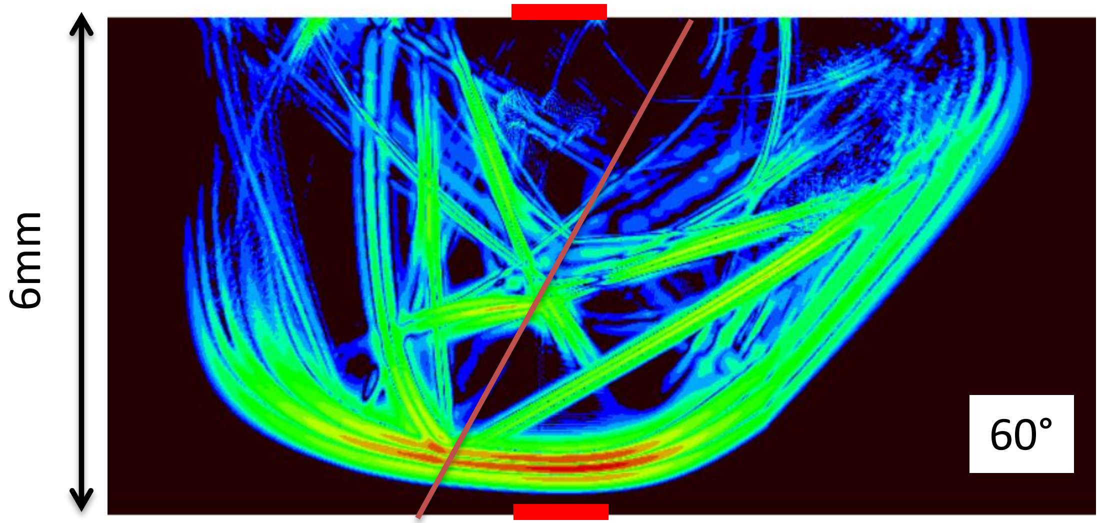


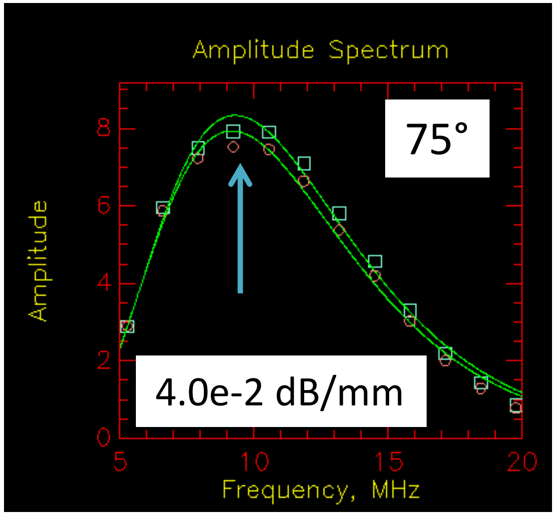


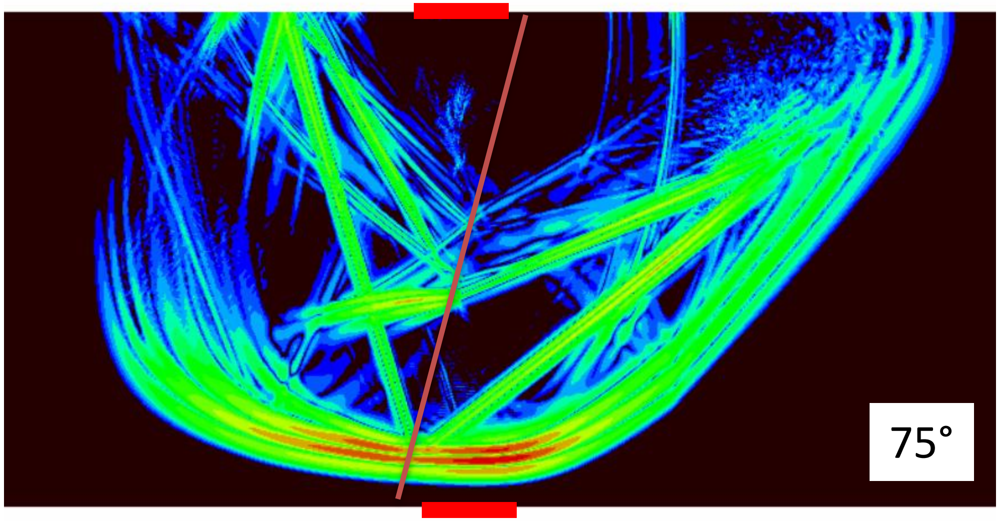
Bi-crystal: anisotropic case

✓ Twin boundary, Reference : Incidence angle 45°



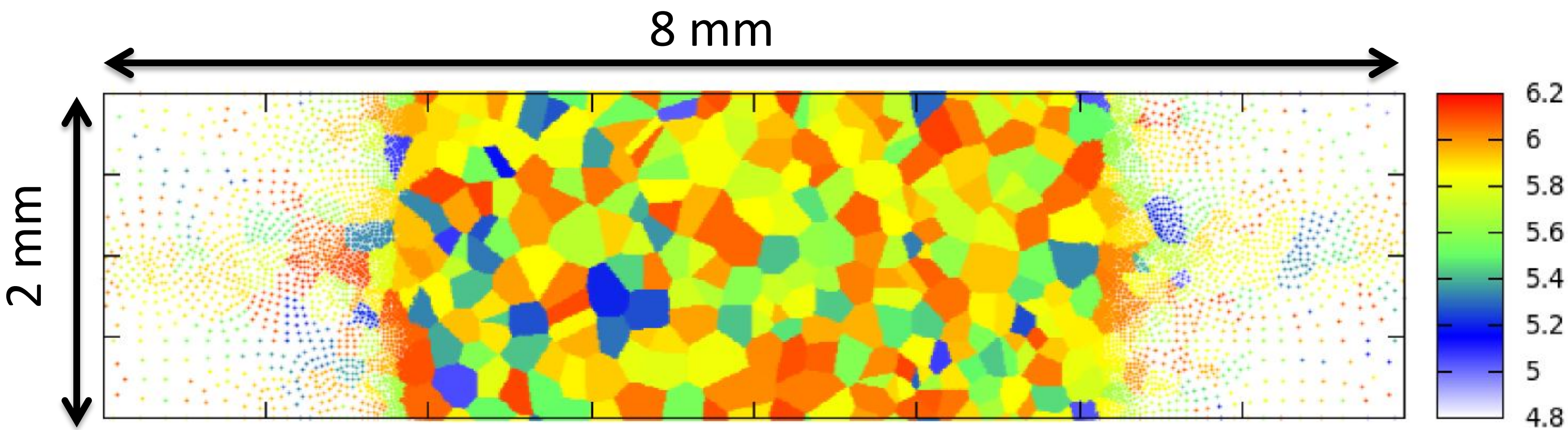






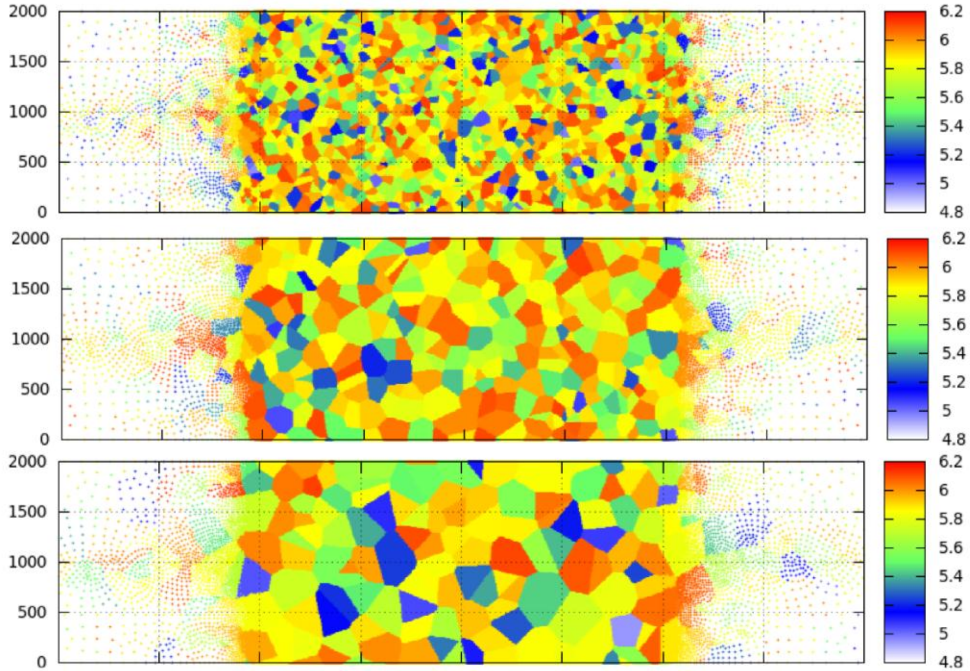
Polycrystalline material

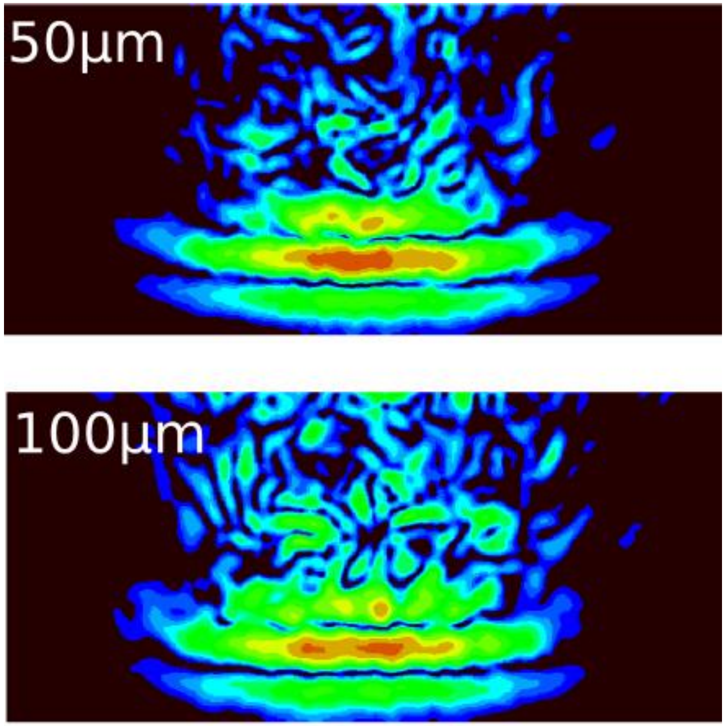
- ✓ Voronoi tessellation
- ✓ Attribution of random orientation (Rodrigues space, axis angle)
- ✓ Attribute rotated stiffness tensors to elements of the mesh for each grain.



Polycrystalline material

✓ Generation of grain size from 20 to 300 µm



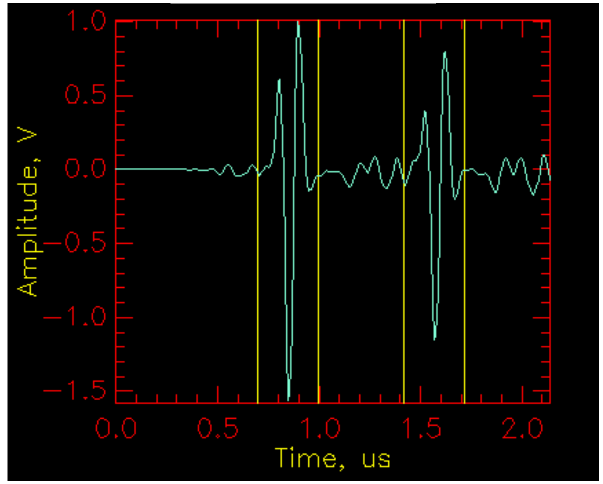


✓ Analysis of ultrasound properties after propagation in the generated structure

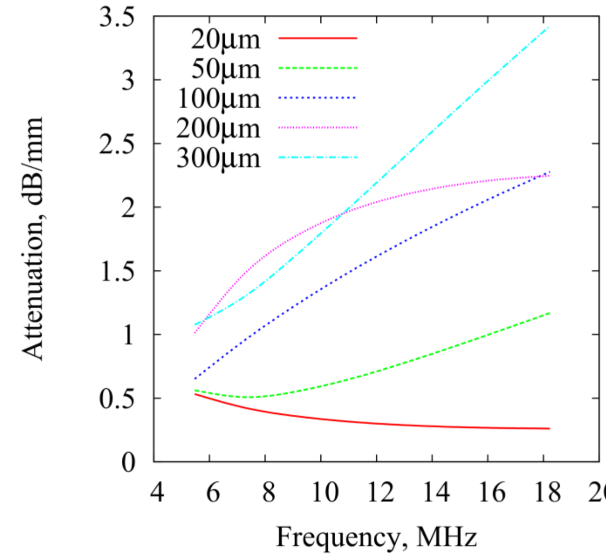
Attenuation and grain size

- ✓ Two echoes
- ✓ Same waveform
- ✓ Larger attenuation for larger grain size
- ✓ Examine the frequency dependence

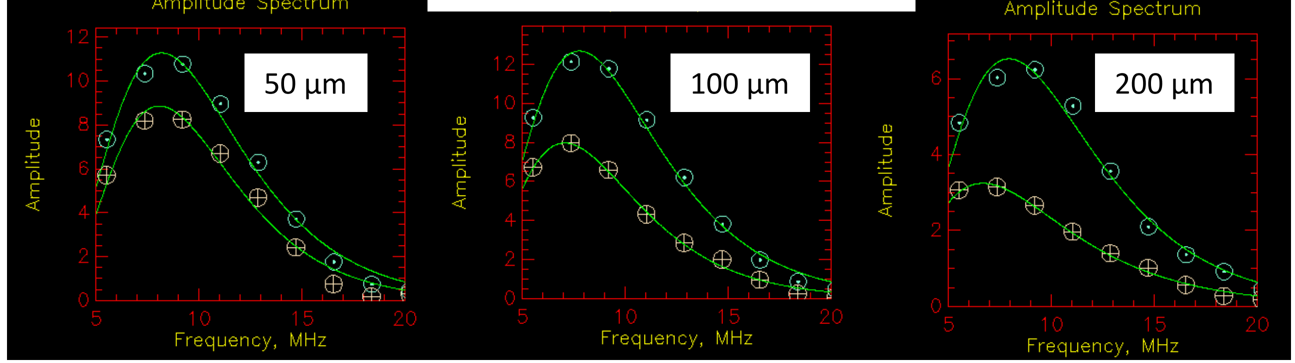
Waveform



Attenuation spectrum



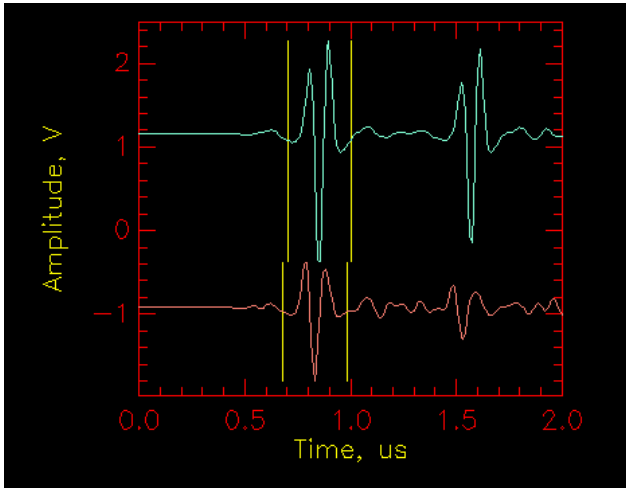
Amplitude spectrum



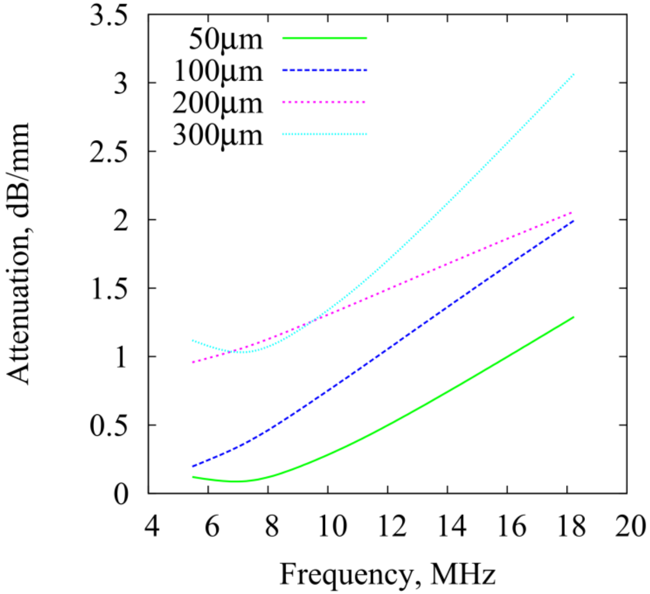
Comparing first echo, Reference 20µm

- ✓ one echoes
- ✓ two waveforms
- ✓ Larger attenuation for larger grain size
- ✓ Examine the frequency dependence

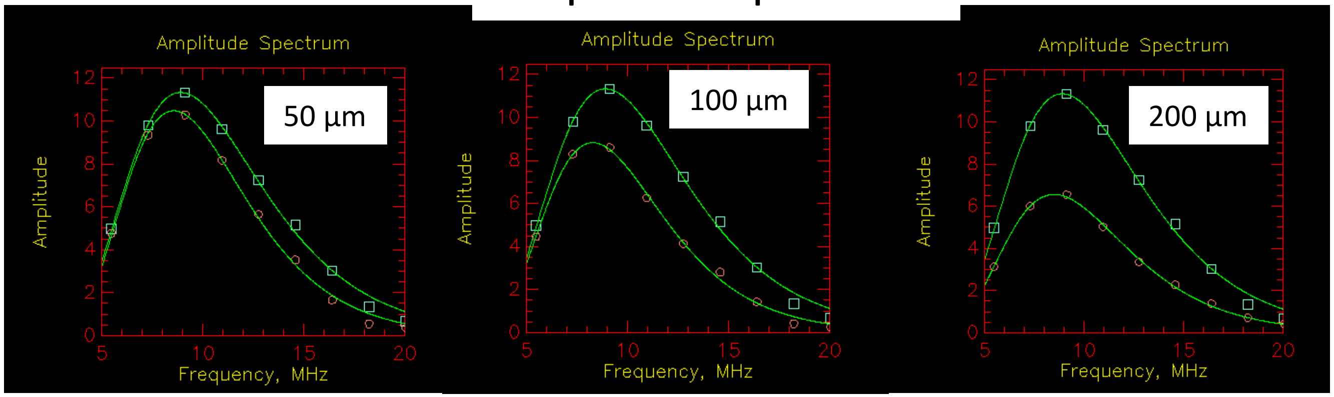
Waveform



Attenuation spectrum

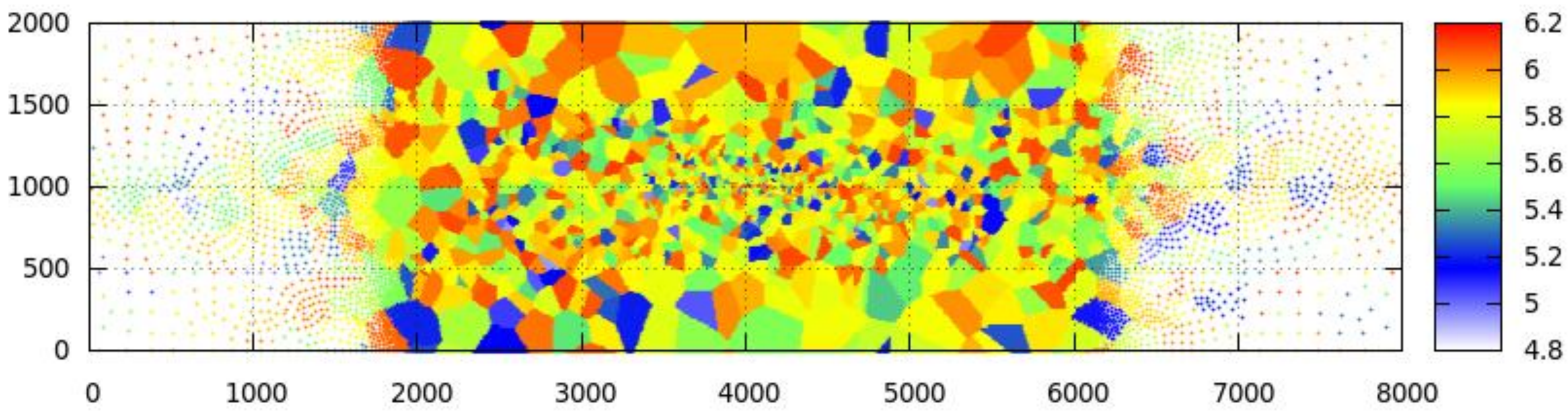


Amplitude spectrum



Grain clusters with various size

- ✓ Play with the pseudo random distribution of center for the Voronoi tessellation
- ✓ Effect of size distribution, cluster of grains, …



Conclusion and future work

- ✓ All three modules (materials properties, FEM, waveform analysis) are validated
- ✓ Need to extend the available bandwidth, high frequencies
- ✓ Compute frequency dependence of attenuation with grain size to compare with scattering theories
- ✓ Evaluate the effect of second phases, presence of cluster of orientations, …