Bulk and lattice waves in PWO: a continuum model

Fabrizio Daví

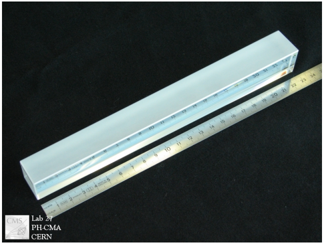
DICEA and ICRYS, Universitá Politecnica delle Marche - Ancona
Crystal Clear Collaboration, CERN - Geneva
PANDA Collaboration, GSI - Darmstadt
on sabbatical leave at IMT-Lucca, Italy

e-Workshop of the IRP Coss&Vita
Advances in ELAstoDYNamics of architected materials and BIOmaterials
Créteil, November 12-13, 2020

Outline

Motivation

- Scintillating crystals are wavelength shifters which convert γ-rays or other ionizating radiation into visible light. They are used in High-Energy Physics (in the CMS experiment at CERN, in the FAIR experiment at GSI in Darmstadt) as well as in advanced and innovative medical imaging devices.
- These crystals are massive, with typical dimensions of centimeters:



$PbWO_4$ (PWO) Scintillator Crystal

- The prolonged exposition to ionizing radiations damages the crystal, displacing atoms and reducing efficiency and transparency of the crystals. There are various techniques of damage recovery, for instant the annealing which requires to remove the crystals from the device with a high risk of mechanical damage of the brittle crystals.
- One alternative and promising technique is the Ultrasound-induced lattice vibration, a technique which can also be applied ”in situ”.
- The goal is to design a tunable and portable laser gun to perform damage recovery ”in situ”.

Ultrasound-Laser based Damage Recovery

In order to optimize the laser energy and frequency we need to understand some basic facts:

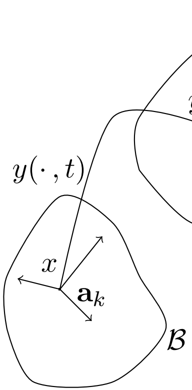
- What are the natural frequencies of the bulk and lattice vibrations;
- How much energy makes the lattice to vibrate and how much is lost in macroscopic vibrations of the bulk crystal;
- What are the lattice vibrations natural modes? And the macroscopic ones?

A continuum mechanics approach

- We do not follow the classical *Lattice dynamics* approach;
- Rather, since we are interested in the coupling between the lattice and bulk dynamics, we follow a continuum mechanics approach;
- We model the crystal as a Continua with Microstructure (Micromorphic Continua, Mindlin, 1964).

F.D.
Wave propagation in micromorphic anisotropic continua with an application to tetragonal crystals.
Mathematics and Mechanics of Solids, (online first, November 12, 2020). DOI: 10.1177/0123456789123456

The micromorphic continuum



$y(\cdot\,,t)$, loc. invertible, orientation pres.

$\mathbf{v} = \dot{y}(x\,,t)$, material velocity

$\mathbf{a}_k(x)$, $k = 1,2,3$, lattice vectors

$\mathbf{G}(\cdot\,,t)$, orientation preserving

$\bar{\mathbf{a}}_k = \mathbf{G}\mathbf{a}_k$ deformed lattice

$$\mathbf{F} = \nabla y = \mathbf{I} + \nabla\mathbf{u}\,, \quad \mathbf{G} = \mathbf{I} + \mathbf{L}\,,$$

$\mathbf{u}$ displacement, $\mathbf{L}$ microdistortion.

Linearized deformation measures

$$\mathbf{E} = \operatorname{sym}\nabla\mathbf{u}\,, \quad \mathbf{M} = \nabla\mathbf{u} - \mathbf{L}\,, \quad \mathsf{G} = \nabla\mathbf{L}\,.$$

Macro- and microscopic balance laws

Microscopic (lattice) balance laws

$$\operatorname{div} \mathsf{H} + \mathbf{S} = \rho \mathbb{J}[\ddot{\mathbf{L}}]\,.$$

- Microstress $\mathsf{H}(y)$;
- Relative stress $\mathbf{S}(y)$;
- Microinertia tensor $\mathbb{J}(y)$;
- Material density $\rho(y)$;

Macroscopic (bulk crystal) balance laws

$$\operatorname{div}(\mathbf{T} + \mathbf{S}) = \rho \dot{\mathbf{v}}\,.$$

- Cauchy stress $\mathbf{T}(y)$;

Linear constitutive relations (Mindlin 1964)

$$
\begin{aligned}
\mathbf{T} &= \mathbb{C}[\mathbf{E}] + \mathbb{D}[\mathbf{M}] + L_c\mathcal{F}[\mathsf{G}]\,,\\
\mathbf{S} &= \mathbb{D}^T[\mathbf{E}] + \mathbb{B}[\mathbf{M}] + L_c\mathcal{G}[\mathsf{G}]\,,\\
\mathsf{H} &= L_c\mathcal{F}^T[\mathbf{E}] + L_c\mathcal{G}^T[\mathbf{M}] + L_c^2\mathfrak{H}[\mathsf{G}]\,.
\end{aligned}
$$

We need to known betweeen 903 independent parameters (Triclinic crystals) and 18 (Isotropic materials).

To make relations dimensionally homogeneous we need to introduce a *Correlation length* L_c, correlated to the non-local effects associated with $\nabla\mathbf{L}$.

Plane bulk and lattice progressive waves

We seek solutions, for the balance laws with linear constitutive relations, of the form:

$$\mathbf{u}(x\,,t) = \mathbf{a}e^{i\sigma}\,, \quad \mathbf{L}(x\,,t) = \mathbf{C}e^{i\sigma}\,, \quad \sigma = \xi\mathbf{x}\cdot\mathbf{m} - \omega t\,,$$

ω is the frequency, $\mathbf{m}$ the direction of propagation, $\xi = \lambda^{-1} > 0$ the wavenumber with λ the wavelength; the amplitudes $\mathbf{a}$ and $\mathbf{C}$ in the general case are complex-valued.

Internal length scales

Two further length scales to make the equations dimensionless:

- *macroscopic length* $L_m > 0$ such that $\mathbf{a} = L_m \mathbf{a}_o$;
- *lattice length* $L_l > 0$, such that $\mathbb{J} = L_l^2 \mathbb{J}_o$.

Introducing the two dimensionless parameters

$$\zeta_1 = \frac{L_c}{L_m}\,, \quad \zeta_2 = \frac{L_l}{L_m}\,,$$

for $\zeta_1 \to 0$ we are considering large samples of crystals; in the limit $L_c \to \infty$ we are zooming into the microstructure. For $\zeta_2 \to 0$ we neglect the contribution of lattice inertia.

Propagation condition

The propagation condition is described by a 12×12 Hermitian matrix A which depends on the constitutive parameters, on the wavenumber ξ and on the dimensionless parameters $\zeta_{1,2}$.

$$(A - \omega^2 J)w = 0\,,$$

$$A \equiv \left[\begin{array}{c|c} \xi^2 \mathbf{A} & \xi^2\zeta_1 \mathsf{P} + i\xi L_m^{-1}\mathsf{Q} \\ \hline \xi^2\zeta_1 \mathsf{P}^T - i\xi L_m^{-1}\mathsf{Q}^T & \xi^2\zeta_1^2\mathbb{A} + L_m^{-2}\bar{\mathbb{B}} \end{array}\right] J \equiv \left[\begin{array}{c|c} \mathbf{I} & \mathbf{0} \\ \hline \mathbf{0} & \zeta_2^2\mathbb{J}_o \end{array}\right] w \equiv \left[\begin{array}{c} \mathbf{a}_o \\ \hline \mathbf{C} \end{array}\right]$$

Propagation condition

We have 12 eigencouples $(\omega_k\,, w_k)$, $k = 1, ..., 12$ with *Dispersion relations* $\xi \mapsto \omega_k(\xi)$.

General results, Lancaster 1964

- There exist 3 Acoustic waves and 9 Optic waves;
- The cut-off frequencies for the Optic waves are the limit as $\xi \to 0$ of the eigenvalues;
- The frequencies for the Acoustic waves are the eigenvalues which goes to zero in the limit for $\xi \to 0$;
- The eigenvectors for $\xi \to 0$ are real.

Limit case 1: $\zeta_{1,2} \to 0$. The long wavelength approximation: macroscopic waves

We "zoom out" and disregard microinertia to recover the classical continuum propagation condition

$$\hat{\mathbf{A}}(\mathbf{m})\mathbf{a}_o = c^2\mathbf{a}_o\,, \quad \omega = c\xi\,, \quad c = v^p = v^g\,,$$

with $\hat{\mathbf{A}}(\mathbf{m})$ a generalization of the classical acoustic tensor:

$$\hat{\mathbf{A}}(\mathbf{m})\mathbf{a}_o = \mathbf{A}(\mathbf{m})\mathbf{a}_o - \mathsf{Q}(\mathbf{m})\mathbb{B}^{-1}\mathsf{Q}^T(\mathbf{m})\mathbf{a}_o = (\mathbb{C} - \mathbb{C}_{micro})[\mathbf{a}_o \otimes \mathbf{m}]\mathbf{m}\,.$$

The (immaginary) lattice modes depend on the macroscopic amplitudes:

$$\mathbf{C} = iL_m\xi\mathbb{B}^{-1}\mathsf{Q}^T(\mathbf{m})\mathbf{a}_o\,,$$

Limit case 2: $L_c \to \infty$ for fixed $L_m \approx L_l$. Microvibrations

In this case we are "zooming into" the crystal to obtain the propagation condition

$$\det(\mathbb{B} - \rho\omega^2\mathbb{J}) = \mathbf{0}\,.$$

and $\mathbf{u}$ reduces to a rigid motion.

We have nine eigencouples $(\omega_k\,,\mathbf{C}_k)$, $k = 1\,,\ldots\,,9$, with real eigentensors and whose eigenvalues represent the cut-off frequencies of $\omega(\zeta)$.

Tetragonal crystals: independent components and lattice modes for PWO, class $4/m$

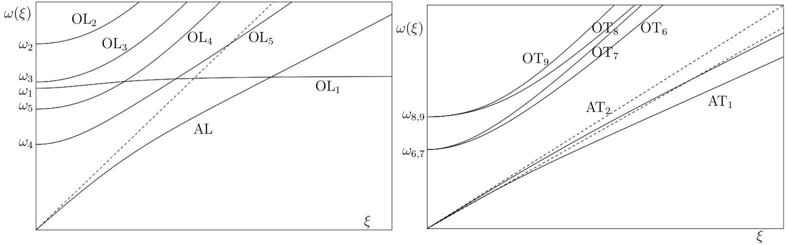
- The matrix A in this case depends on 43 components;
- The lattice modes are a combination of two dilatations $\mathbf{D}_1$ (non-uniform dilatation) and $\mathbf{D}_2$ (plane strain orthogonal to c, pure dilatation along c), two shears $\mathbf{S}_1$ (in the plane orthogonal to c and $\mathbf{S}_2$ (between c and an orthogonal direction and two rigid rotations $\mathbf{R}_1$ (about c) and $\mathbf{R}_2$ (about a direction orthogonal to c);
- The bulk modes are a longitudinal and two transverse waves.

Eigenvalues and eigenmodes

- One Acoustic wave associated with a macroscopic displacement along c and a combination of the modes $\mathbf{D}_1$, $\mathbf{S}_1$ and $\mathbf{R}_1$, which for $\xi = 0$ reduced to a macroscopic longitudinal wave; (AL)
- Two Acoustic waves associated with a macroscopic displacement orthogonal to c, coupled a combination of the modes $\mathbf{S}_2$ and $\mathbf{R}_2$. For $\xi = 0$ these waves reduce to two macroscopic orthogonal transverse waves; ($\mathrm{AT}_{1,2}$)

- Four Optic waves associated with a macroscopic displacement along c and with a microdistortion which combines the modes $\mathbf{D}_1$, $\mathbf{S}_1$ and $\mathbf{R}_1$; (OL$_{1,2,4,5}$)
- One Optic wave associated with a macroscopic displacement along c and with a combination of the modes $\mathbf{D}_2$ and $\mathbf{R}_1$; (OL$_3$)
- Four Optic waves associated with a macroscopic displacement orthogonal to c coupled with a combination of the $\mathbf{S}_2$ and $\mathbf{R}_2$ modes. (OT$_{7,8,10,11}$)

Dispersion relations



Further developments

- Design experiments to evaluate the 43 independent components;
- Identify these components by homogenezation techniques from lattice dynamics;
- Evaluate the amount of energy which is lost in acoustic waves;
- Study the best lattice modes to obtain the maximum effect.

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Es gibt nichts mehr praktisch als eine gute theorie

(L. Prandtl 1875-1953)

Thanks for the attention!