# 3D Elastodynamics

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## 1 Model

The elastodynamic equation for the local mechanical displacement $\mathbf{u}$ in anisotropic crystals describes the relationship between the displacement of a point in a crystal and the external forces acting on it.

$$\rho\frac{\partial^2 u_i}{\partial t^2} + \beta\frac{\partial u_i}{\partial t} = \boldsymbol{\nabla}_j \sigma_{ij} + f_i \tag{1}$$

Here $\rho$ is density, $\beta$ is damping constant, $\sigma_{ij}$ is strain tensor components, $f_i$ is a force density. This second order differential equation may be reduced to system of 1st order equations. Which can be expressed thru velocities $v_i = \partial u_i/\partial t$ and stresses $\sigma_{ij} = c_{ijkl}\epsilon_{kl}$

$$\begin{cases} \rho\frac{\partial v_i}{\partial t} + \beta v_i = \boldsymbol{\nabla}_j \sigma_{ij} + f_i \\ \frac{\partial \sigma_{ij}}{\partial t} = c_{ijkl}\frac{1}{2}(\frac{\partial v_k}{\partial l} + \frac{\partial v_l}{\partial k}) \end{cases} \tag{2}$$

Now we have system of nine first order DE which we will solve using leapfrog scheme[1,2,3]. Velocities and stresses are shifted in space and time in half of integrating steps $di$, $dt$. Let's consider a cubic symmetry for simplicity, then equation of state reads in Voigt notation $\sigma = c\epsilon$, where $c$ is an elastic matrix

$$c = \begin{pmatrix} c11 & c12 & c12 & 0 & 0 & 0 \\ c12 & c11 & c12 & 0 & 0 & 0 \\ c12 & c12 & c11 & 0 & 0 & 0 \\ 0 & 0 & 0 & c44 & 0 & 0 \\ 0 & 0 & 0 & 0 & c44 & 0 \\ 0 & 0 & 0 & 0 & 0 & c44 \end{pmatrix} \tag{3}$$

To implement free boundary conditions (FBC) one needs to state that vacuum does not apply pressure on the boundary. FBC in direction normal to $i$ $\{\sigma_{ij} = 0\}_j$ reads as

$$\begin{cases} \partial v_i/\partial i = -c12/c11(\partial v_j/\partial j + \partial v_k/\partial k) \\ \partial v_j/\partial i = -\partial v_i/\partial j \end{cases} \tag{4}$$

To obtain an open BC let's rewrite (2) with respect to $\boldsymbol{\Phi}$ vector which is constructed as $(v_x, v_y, v_z, \sigma_{xx}, \sigma_{yy}, \sigma_{zz}, , \sigma_{yz}, \sigma_{xz}, \sigma_{xy})^T$. This hyperbolic system has 9 characteristic curves along which Riemann invariants are conserved and may be inflowing or outflowing at boundaries. These invariants are widely used in mathematics to deal with hyperbolic equations.

$$\frac{\partial \boldsymbol{\Phi}}{\partial t} = \beta\boldsymbol{\Phi} + \sum_i A_i\frac{\partial \boldsymbol{\Phi}}{\partial i} + \boldsymbol{f} \tag{5}$$

for example $Ax$ has form

$$\begin{pmatrix} 0 & 0 & 0 & 1/\rho & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/\rho \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/\rho & 0 \\ c_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & c_{44} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c_{44} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6}$$

Diagonalization of this system as in [4] leads to 9 eigenvalues $\lambda_n$ and eigenvectors $W_n$. Rieman invariants or new characteristic variables vector has form $\boldsymbol{\phi} = E^{-1}\boldsymbol{\Phi}$, where E is matrix constructed from eigenvectors of matrix $A_i$. Now we define characteristic amplitudes as $L_n = \lambda_n\phi_n/\partial i$ where $i$ is direction normal to open boundary. And finally set of $L_n = 0$ is open BC. These conditions take form

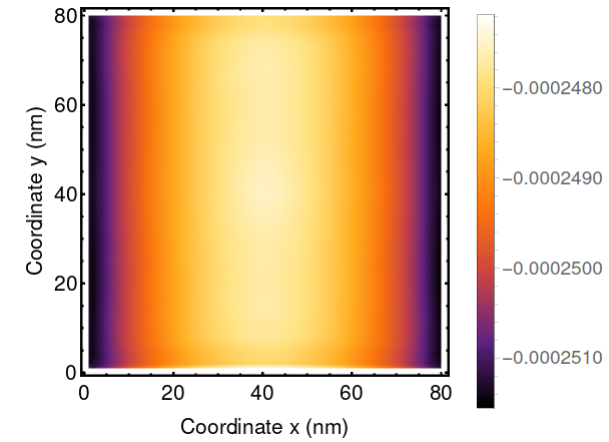
$$\begin{cases} \frac{\partial V_i}{\partial i} = \pm\frac{1}{\sqrt{c_{11}\rho}}\frac{\sigma_{ii}}{\partial i} \\ \frac{\partial V_j}{\partial i} = \pm\frac{1}{\sqrt{c_{44}\rho}}\frac{\sigma_{ij}}{\partial i} \end{cases} \tag{7}$$

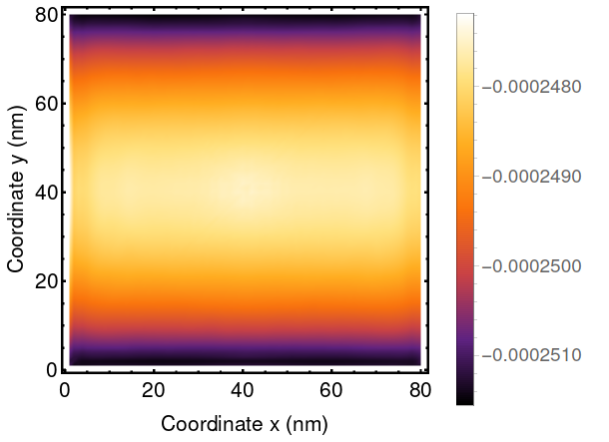
Here sign $\pm$ denotes to right and left boundaries.

# 2 Results

## 2.1 Poison's ratio

First of all let's simulate a compression of CoFe cube with cell numbers $l_x = l_y = l_z = 80$ and cell sizes $dx = dy = dz = 3$ nm. We apply constant $f_z$ at upper surface $z = lz$ of cube and fix $v_z = 0$ at lower surface $z = 0$ and let all the rest boundaries be free. Stationary spatial distributions of strains at layer number $lz/2$ are shown on fig.1. This graph shows the distribution of stresses that corresponds to ground state. FBC allow normal strain relaxation thru the tangential terms (shear stresses). Poison's ratio, also known as the lateral strain coefficient, is a measure of the relationship between the change in a material's cross-sectional area and its longitudinal length when it is subjected to an external load. It is a dimensionless number typically between 0 and 0.5. Poison's ratio can be used to determine the amount of perpendicular strain that occurs in relation to the normal strain. Analytical Poison's ratio $c_{12}/(c_{11}+c_{12})$ and resulting $\epsilon_{xx}/\epsilon_{zz}$ at point $(lx/2, ly/2, lz/2)$ are -0.372133 and -0.372881 respectively.



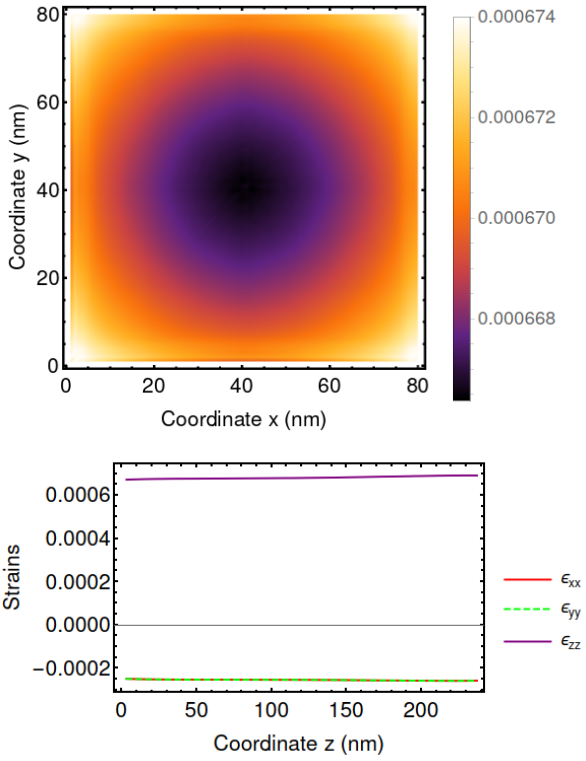




Fig. 1 $\epsilon_{xx}(x,y)$ , $\epsilon_{yy}(x,y)$ , $\epsilon_{zz}(x,y)$, $\epsilon_{xx,yy,zz}(z)$

## 2.2 Isotropic inplane strains

Now let's consider a case when we have an applied inplane stretching forces $f_x$ and $f_y$ at bottom $(z = 0)$ of CoFe film with geometry $lx = ly = 100$, $lz = 2$, $dx = dy = 3$ nm, $dz = 1.5$ nm. Forces are calculated as $f_i = \sigma_{ii}^{ext}/\Delta i$ with chosen external strains $\epsilon_{xx}^{ext} = \epsilon_{yy}^{ext} = 1\%$ and $\Delta i$ is a computational cell size. All directions of the plotted strain functions intersect at the point $(l_x/2, l_y/2, l_z/2)$. The results are shown on fig 2.

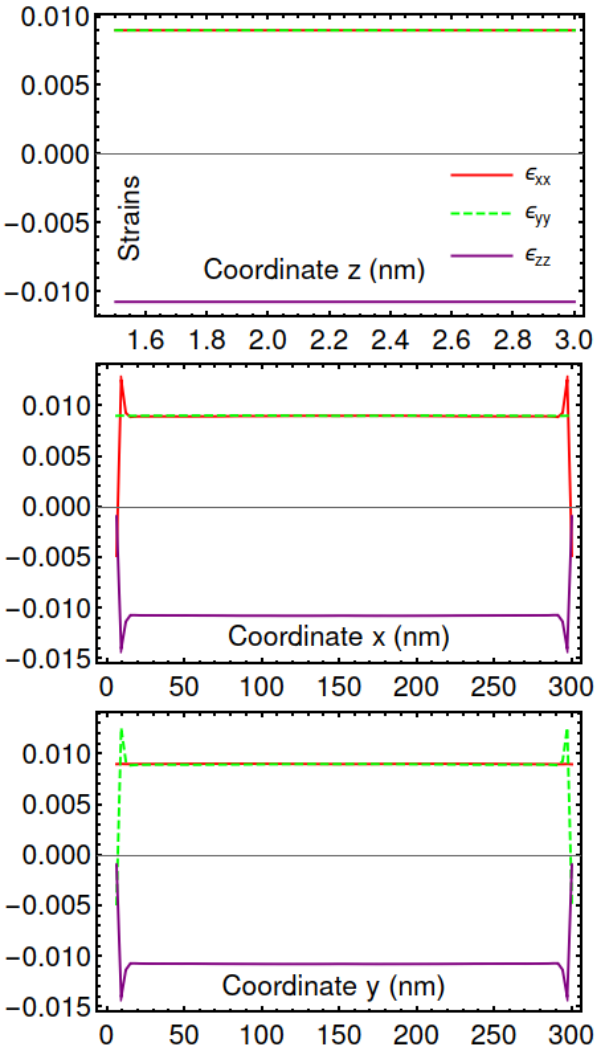



Fig. 2 $\epsilon(x, y, z)$ $l_x = l_y = 100$, $l_z = 2$, $dx = dy = 3$ nm, $dz = 1.5$ nm

Now let's consider a geometry $l_x = l_y = 100$, $l_z = 20$, $dx = dy = 3$ nm, $dz = 1.5$ nm. The results are shown on fig 3.

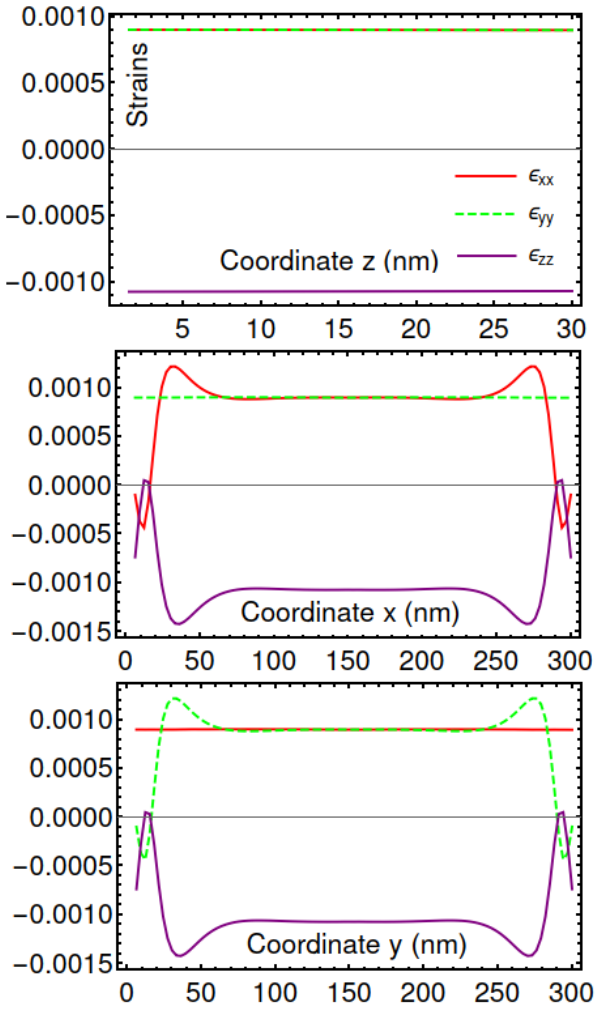



Fig. 3 $\epsilon(x, y, z)$ $l_x = l_y = 100$, $_lz = 20$, $dx = dy = 3$ nm, $dz = 1.5$ nm

Simulation with elongated shape CoFe crystal with $lx = ly = 10$, $lz = 200$, $dx = dy = dz = 3$ nm. Fig 4 illustrates the result.

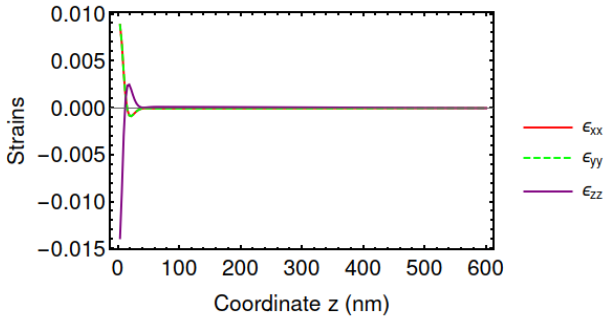



Fig. 4 $\epsilon(z)$ $l_x = l_y = 10$, $l_z = 200$, $dx = dy = dz = 3$ nm

Let's see what happens if we apply isotropic inplane strains at MgO-CoFe-Pt structure with $l_x = l_y = 100$, $l_z = 21$, $dx = dy = 3$ nm, $dz = 0.5$ nm.

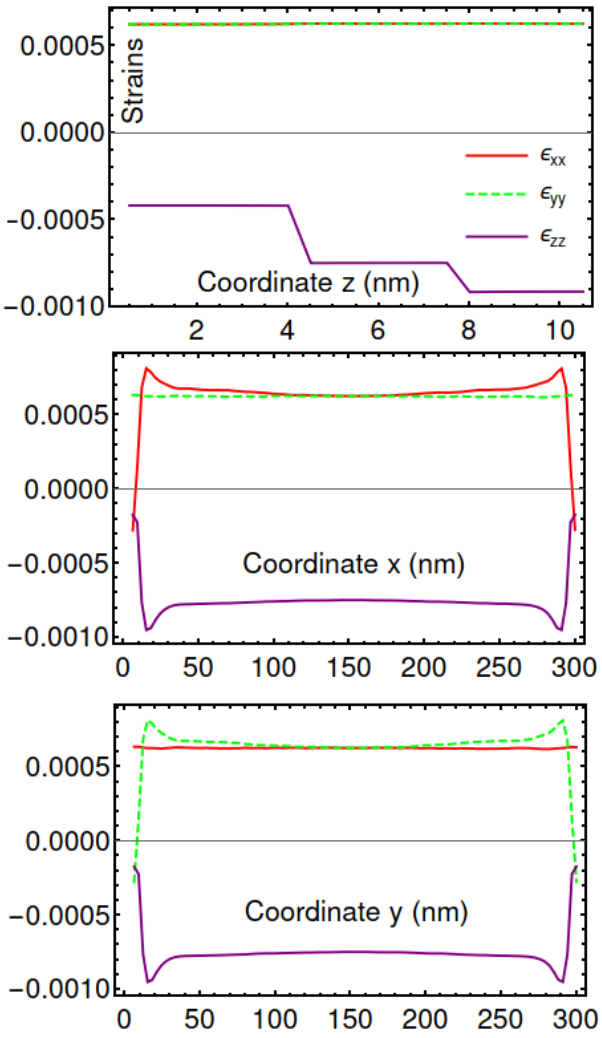



Fig. 5 MgO-CoFe-Pt structure

## 2.3 Dynamics

In order to check absolute absorption condition and relation of amplitudes of waves passing the interface between different materials we apply a time-dependent values of stresses at $z = 0$:

$$\begin{cases} \sigma_{xx} = \sigma_{yy} = c_{12}\epsilon_{zz} \sin 2\pi\nu t \\ \sigma_{zz} = c_{11}\epsilon_{zz} \sin 2\pi\nu t \\ \sigma_{xy} = \sigma_{xz} = \sigma_{yz} = 0 \end{cases} \tag{8}$$

These conditions allow us to simulate a longitudinal waves with constant wave front in $xy$ plane. Layer number $z = l_z/2$ is interface, where region $z \leq l_z/2$ is MgO and $z > l_z/2$ is CoFe crystal. We apply an open BC at $z = lz$ surface and free BC to all the rest surfaces of 3-dimensional waveguide with $l_x = l_y = 10$, $l_z = 800$, $dx = dy = dz = 5$ nm. Fig 6 shows the results obtained with simulation using $dt = 10^{-15}$ s and applied frequency is 10 GHz. Wave lengths of MgO and CoFe are 886 and 558 nm.

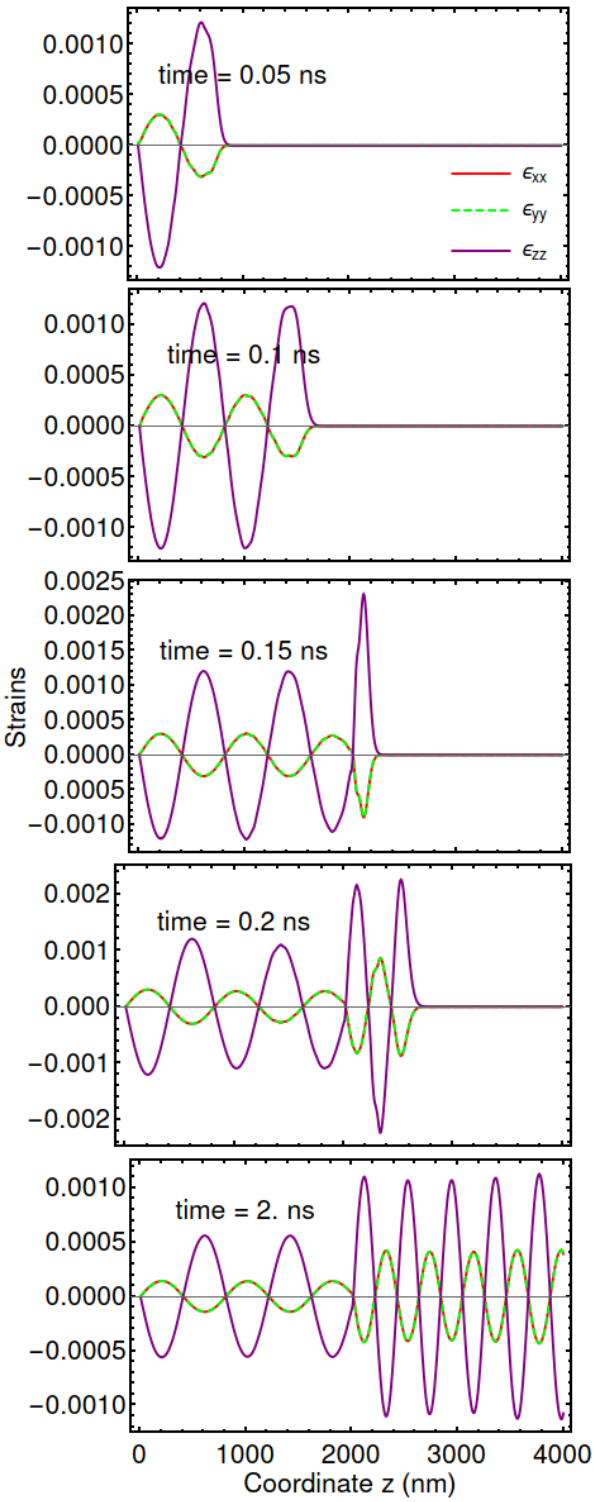



Fig. 6 MgO-CoFe weveguide time series.

Spatial distributions of $\boldsymbol{u}$ along z axis are shown on fig. 7. Analytical value of ratio of misfits is $u_{CoFe}/u_{MgO} = Z_{MgO}/(Z_{MgO} + Z_{CoFe}) = 0.798$, where Z equals wave velocity times mass density. Numerical value of $u_{CoFe}/u_{MgO} = 0.815$.

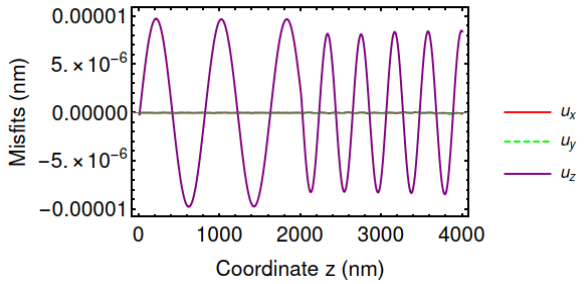



Fig. 7 MgO-CoFe weveguide misfits amplitudes.

### 2.4 Impulse reflection from MgO-CoFe interface

Finally let's consider a structure with geometry from 2.3 but now we will generate an impulse at $z = 0$ boundary. In order to study $\boldsymbol{u}$ reflected from interface open BC will be applied at all other surfaces. This is a semi infinite crystal case and we expect $\boldsymbol{u}$ to be distributed uniformly in $xy$ plane. Impulse has form

$$\begin{cases} \epsilon_{zz} = 0.001 & t \leq 0.01ns \\ \epsilon_{zz} = 0 & t > 0.01ns \end{cases}$$

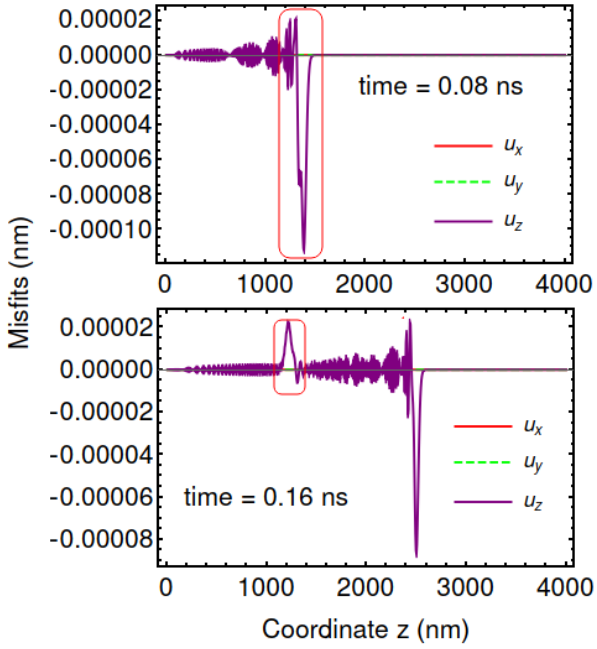



Fig. 8 MgO-CoFe infinite crystal misfits amplitudes.

Ratio of primary and reflected amplitudes sdfgdrgh $(Z_{MgO} - Z_{CoFe})/(Z_{MgO} + Z_{CoFe}) = -0.2$. And numerical value of ratio is -0.2, what can be seen from time series shown on fig 8.

## References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[3] D.C. Calvo and K.E. Rudd and M. Zampolli and W.M. Sanders and L.D. Bibee "Simulation of acoustic scattering from an aluminum cylinder near a rough interface using the elastodynamic finite integration technique", Wave Motion,2010,0165-2125,https://doi.org/10.1016/j.wavemoti.2010.05.002

[4] https://hal.inria.fr/inria-00134856/document