3D Elastodynamics

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1 Model

The elastodynamic equation for the local mechanical displacement $\boldsymbol{u}$ is written as

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

Which can be expressed using expressions for 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. Free BC in direction normal to i $\{\sigma_{ij}=0\}_j$ leads to

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

(3)

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.

$$\frac{\partial\boldsymbol{\Phi}}{\partial t}=\beta\boldsymbol{\Phi}+\sum_i A_i\frac{\partial\boldsymbol{\Phi}}{\partial i}+\boldsymbol{f} \tag{4}$$

for example Ax has form

$$\begin{pmatrix}0&0&0&1/\rho&0&0&0&0&0\\0&0&0&0&0&0&0&0&1/\rho\\0&0&0&0&0&0&0&1/\rho&0\\c_{11}&0&0&0&0&0&0&0&0\\c_{12}&0&0&0&0&0&0&0&0\\c_{12}&0&0&0&0&0&0&0&0\\0&0&0&0&0&0&0&0&0\\0&0&c_{44}&0&0&0&0&0&0\\0&c_{44}&0&0&0&0&0&0&0\end{pmatrix}. \tag{5}$$

Diagonalization of this system as in [4] leads to 9 eigenvalues λ_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

$$\begin{cases}\frac{\partial V_i}{\partial i}=\pm\frac{1}{\sqrt{c_{11}\rho}}\frac{\sigma_{ii}}{\partial i}\\ \frac{\partial V_j}{\partial i}=\pm\frac{1}{\sqrt{c_{44}\rho}}\frac{\sigma_{ij}}{\partial i}\end{cases} \tag{6}$$

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

2 Results

2.1 Poison's coefficient

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.

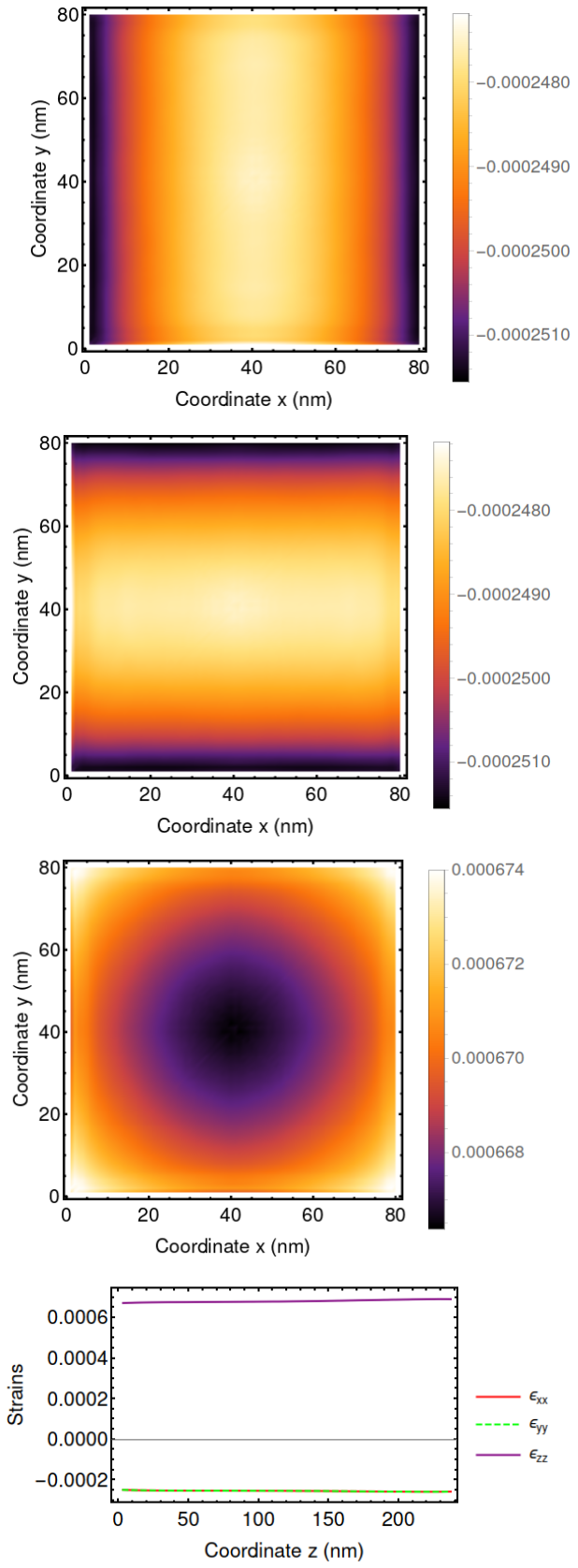

Fig. 1 $\epsilon_{xx}(x,y)$, $\epsilon_{yy}(x,y)$, $\epsilon_{zz}(x,y)$, $\epsilon_{xx,yy,zz}(z)$

Analytical Poison's coefficient $c_{12}/(c_{11}+c_{12})$ and resulting $\epsilon_{xx}/\epsilon_{zz}$ at point $(lx/2, ly/2, lz/2)$ are -0.372133 and -0.372881 respectively.

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 Δi 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.

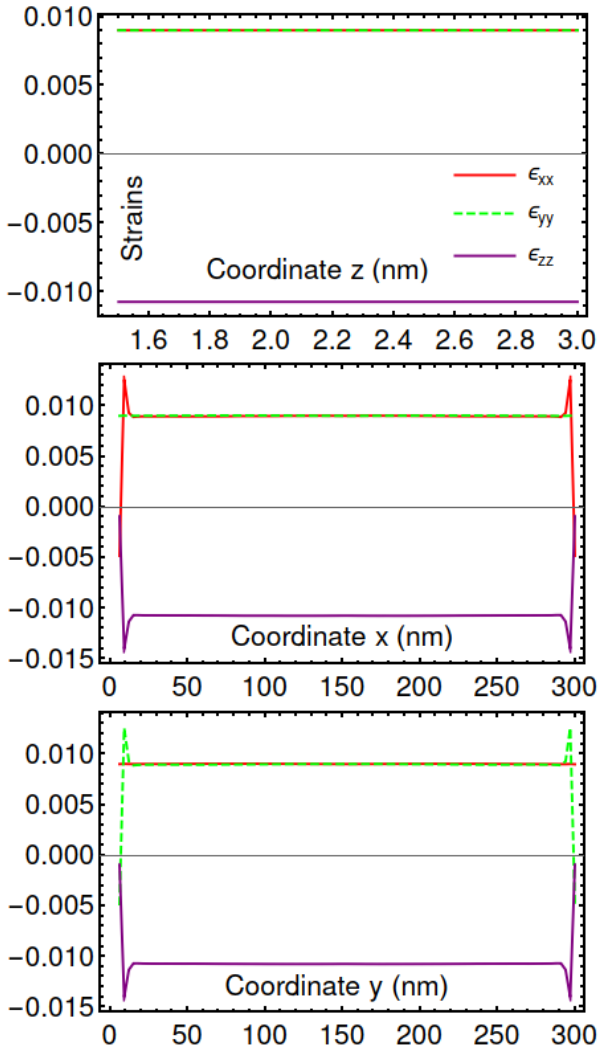

Fig. 2 $\epsilon(x,y,z)$ $l_x = l_y = 100$, $l_z = 2$, $dx = dy = 3$ nm, $dz = 1.5$ nm

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.

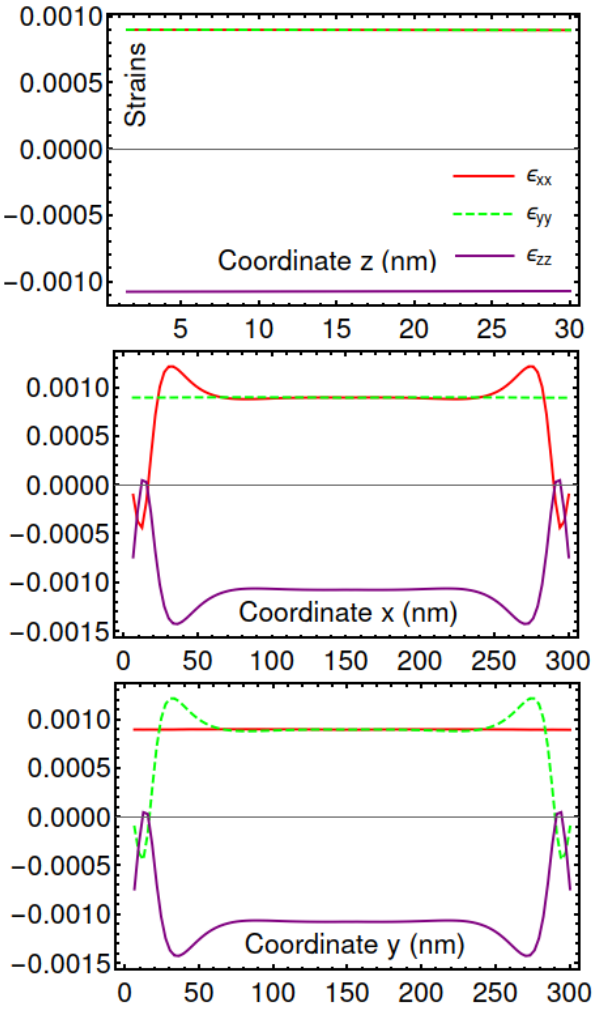

Fig. 3 $\epsilon(x, y, z)$ $l_x = l_y = 100$, $_lz = 20$, $dx = dy = 3$ nm, $dz = 1.5$ nm

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

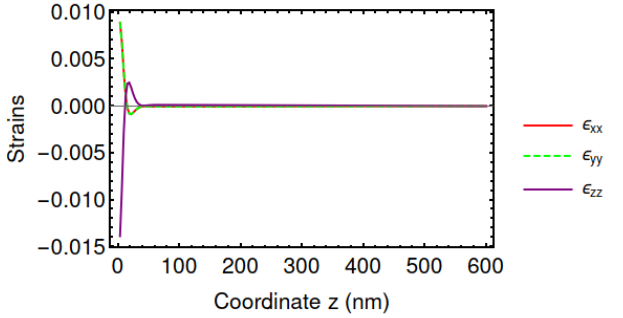

Fig. 4 $\epsilon(z)$ $l_x = l_y = 10$, $l_z = 200$, $dx = dy = dz = 3$ nm

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.

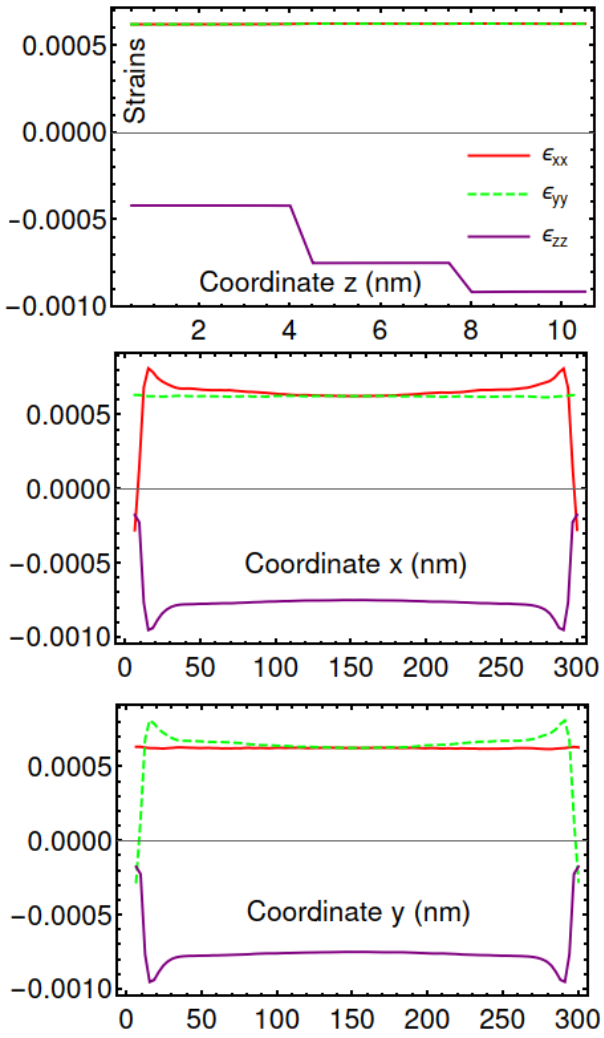

Fig. 5 MgO-CoFe-Pt structure

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 $z = 0$:

$$\begin{cases} \sigma_{xx} = \sigma_{yy} = c_{12}\epsilon_{zz} \sin 2\pi\nu t \\ \sigma_{zz} = c_{11}\epsilon_{zz} \sin 2\pi\nu t \\ \sigma_{xy} = \sigma_{xz} = \sigma_{yz} = 0 \end{cases} \quad (7)$$

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.

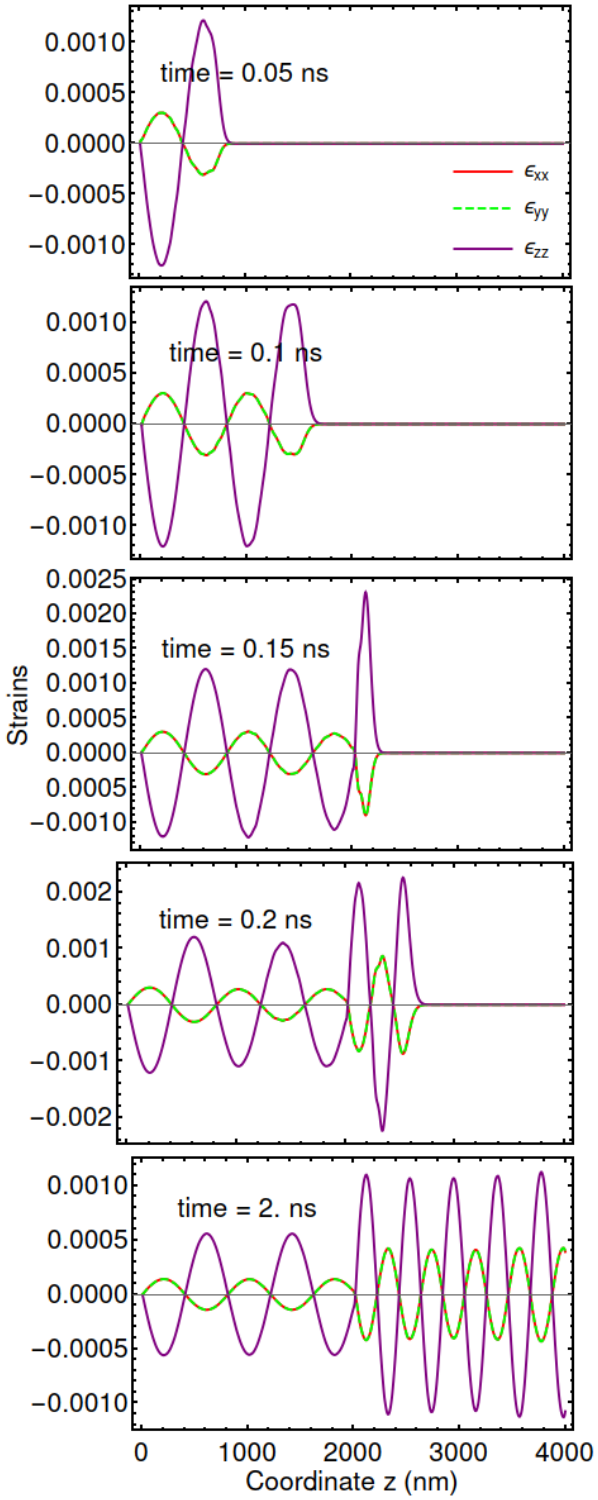

Fig. 6 MgO-CoFe weveguide time series.

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 $u_{CoFe}/u_{MgO} = 0.815$.

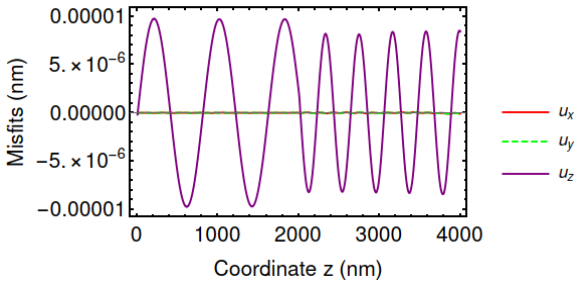

Fig. 7 MgO-CoFe weveguide misfits amplitudes.

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

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

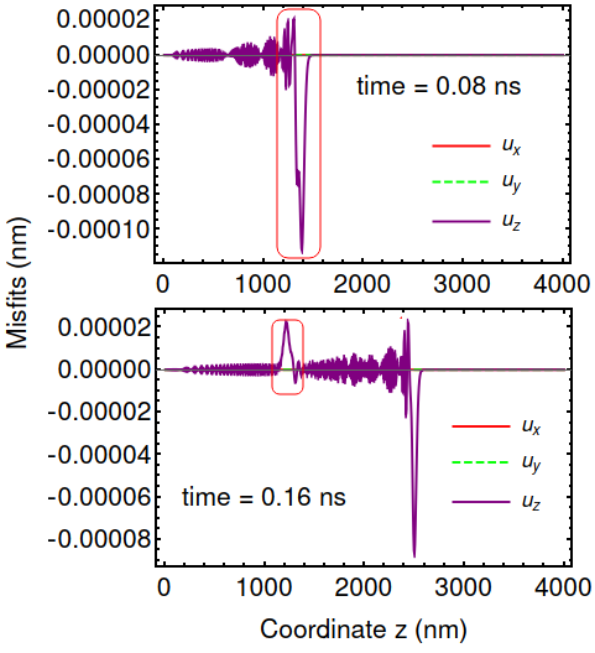

Fig. 8 MgO-CoFe infinite crystal misfits amplitudes.

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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