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# Numerical Simulation of Piezoelectric Effect under Ultrasound Irradiation: Consideration of the Conductivity

# 超音波照射下での圧電効果の数値シミュレーション：導電性の考慮

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## 1. Introduction

Bone formation can be driven by mechanical loads given to the bone, and the bone structure can be adapted to the mechanical condition.[1] This mechanism has been applied to the clinical healing of bone fracture by the irradiation of low-intensity pulsed ultrasound (LIPUS).[2] Moreover, the bone formation can be accompanied by the piezoelectric effect.[3] To realize more effective method of the ultrasound irradiation for bone formation, the electric fields induced in the bone should be understood. However, the electric signal in the bone is difficult to detect because it is very small. In such a case, numerical simulations can be helpful.

In the previos study,[4] a piezoelectric finite-difference time-domain (PE-FDTD) method was used to simulate the electric fields in a human femur under ultrasound irradiation. However, the conductivity of the bone was not considered, and therefore, the bone was regarded as a perfect insulator. In this study, the PE-FDTD simulation with consideration of the conductivity was performed to investigate its effect.

## 2. Simulation Method

In the PE-FDTD method, a motion equation and piezoelectric constitutive equations were used and are shown in Eqs. (1)–(4).

$$\rho \frac{\partial \dot{u}_i}{\partial t} = \frac{\partial \tau_{ii}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \tau_{ik}}{\partial x_k} \tag{1}$$

$$\begin{aligned} \frac{\partial \tau_{ii}}{\partial t} = (\lambda + 2\mu)\frac{\partial \dot{u}_i}{\partial x_i} + \lambda \frac{\partial \dot{u}_j}{\partial x_j} + \lambda \frac{\partial \dot{u}_k}{\partial x_k} - e_{ii}\frac{\partial E_i}{\partial t} \\ - e_{ji}\frac{\partial E_j}{\partial t} - e_{ki}\frac{\partial E_k}{\partial t} \end{aligned} \tag{2}$$

$$\begin{aligned} \frac{\partial \tau_{jk}}{\partial t} = \mu\left(\frac{\partial \dot{u}_j}{\partial x_k} + \frac{\partial \dot{u}_k}{\partial x_j}\right) - e_{il}\frac{\partial E_i}{\partial t} - e_{jl}\frac{\partial E_j}{\partial t} \\ - e_{kl}\frac{\partial E_k}{\partial t} \end{aligned} \tag{3}$$

$$\begin{aligned} \varepsilon_{ii}\frac{\partial E_i}{\partial t} = -e_{ii}\frac{\partial \dot{u}_i}{\partial x_i} - e_{ij}\frac{\partial \dot{u}_j}{\partial x_j} - e_{ik}\frac{\partial \dot{u}_k}{\partial x_k} \\ - \frac{e_{il}}{2}\left(\frac{\partial \dot{u}_j}{\partial x_k} + \frac{\partial \dot{u}_k}{\partial x_j}\right) - \frac{e_{im}}{2}\left(\frac{\partial \dot{u}_k}{\partial x_i} + \frac{\partial \dot{u}_i}{\partial x_k}\right) \\ - \frac{e_{in}}{2}\left(\frac{\partial \dot{u}_i}{\partial x_j} + \frac{\partial \dot{u}_j}{\partial x_i}\right) + \frac{\partial D_i}{\partial t} \end{aligned} \tag{4}$$

Here, $i, j, k = 1, 2, 3$, and $l, m, n = 4, 5, 6$. In these equations, $\dot{u}_i$ (dot denotes the time derivative) is the particle velocity in the $i$-direction, $\tau_{ii}$ is the normal stress in the $i$-direction, $\tau_{jk}$ ($j \neq k$) is the shear stress on the $j$–$k$ plane, $E_i$ is the electric field, and $D_i$ is the electric displacement. $\rho$ is the density, $\lambda$ and $\mu$ are the first and second Lamé coefficients, respectively, $e_{ij}$ (containing $i = j$) is the piezoelectric constant, and $\varepsilon_{ii}$ is the dielectric constant.

The time derivative of the electric displacement, that is the current density, was assumed to be zero in the previous study,[4] but Eq. (5) was used in this study.

$$\frac{\partial D_i}{\partial t} = -\sigma_i E_i \tag{5}$$

Here, $\sigma_i$ is the conductivity. In the PE-FDTD algorism, the values of $\dot{u}_i$ and $D_i$ and the values of $\tau_{ii}$, $\tau_{ij}$, and $E_i$ were alternatively updated.

The PE-FDTD simulation was performed for the piezoelectric ceramics of $Pb(Zr,Ti)O_3$ (PZT). In the simulation model of Fig. 1, the water region was $10 \times 10 \times 15$ mm$^3$, in the middle of which the PZT region of $10 \times 10 \times 5$ mm$^3$ was allocated. The 3-direction corresponded to the thickness direction, which was parallel to the ultrasound transmission. The elastic and piezoelectric parameter values of the PZT and water are listed in Table I. In order to investigate the effect of the conductivity, three conductivity values of $\sigma_i = 10^{-6}$, $10^{-2}$, and $10^{-1}$ S/m, which corresponded to the values for an insulator, water, and cortical bone, respectively, were used for the PZT. As the input, a single sinusoid multiplied by a Hanning window, which had a center frequency of 1 MHz, was given to the particle displacement of $u_3$ on the transmitting surface. As the output, the sum of the normal stress of $\tau_{33}$ on the

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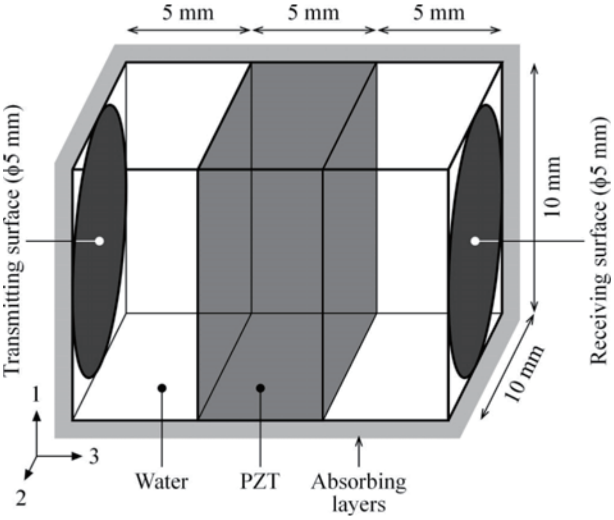

Fig. 1 Simulation model for piezoelectric effect in PZT induced by an ultrasound wave.

Table I Elastic and piezoelectric parameter values of PZT and water used in PE-FDTD simulation.

| | PZT | Water |
|---|---|---|
| First Lamé coefficient $\lambda$ (GPa) | 81.1 | 2.2 |
| Second Lamé coefficient $\mu$ (GPa) | 24.4 | 0 |
| Density $\rho$ (kg/m$^3$) | 7620 | 1000 |
| Piezoelectric constant $e_{31}$, $e_{32}$ (C/m$^2$) | -13.0 | 0 |
| $e_{33}$ (C/m$^2$) | 23.1 | |
| $e_{15}$, $e_{24}$ (C/m$^2$) | 14.4 | |
| Dielectric constant $\varepsilon_{11}$, $\varepsilon_{22}$ (nF/m ) | 20.1 | 0.7 |
| $\varepsilon_{33}$ (nF/m ) | 18.9 | |
| Conductivity $\sigma_1$, $\sigma_2$, $\sigma_3$ (S/m) | $\begin{cases}10^{-6}\\10^{-2}\\10^{-1}\end{cases}$ | $10^{-2}$ |

receiving surface and the electric field of $E_3$ at the center point of the PZT were calculated. The former corresponded to the ultrasound signal propagating through the PZT.

## 3. Simulated Results

Figures 2 and 3 show the simulated waveforms of the ultrasound signal through the PZT and the electric field of $E_3$ at the center of the PZT, respectively. In both figures, the black, dark gray, and light gray lines illustrate the waveforms for the conductivity values of $\sigma_i$ = $10^{-6}$, $10^{-2}$, and $10^{-1}$ S/m, respectively. In Fig. 2, as the conductivity increases, the ultrasound speed in the PZT becomes slightly slower. In the previous study,[4] it was shown that the speed increased with the piezoelectricity. Therefore, the slower speed means the smaller piezoelectric effect. In fact, the electric field of $E_3$ in Fig. 3 decreases with the conductivity. On the other hand, the ultrasound amplitude in Fig. 2 decreases with the conductivity, although the previous study[4] showed the decrease in the amplitude with the piezoelectricity. Accordingly, it is concluded that the conductivity cannot only prevent the piezoelectric effect.

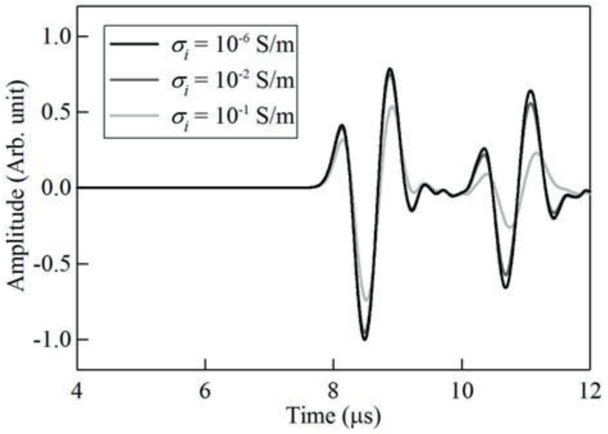

Fig. 2 Simulated waveforms of ultrasound signal propagating through PZT at three values of conductivity, $\sigma_i$.

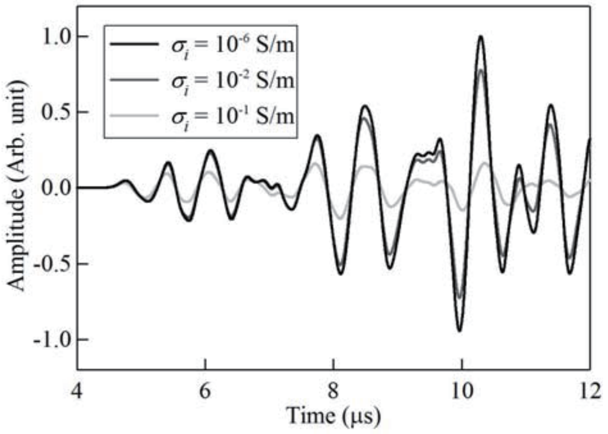

Fig. 3 Simulated waveforms of electric field of $E_3$ in PZT at three values of conductivity, $\sigma_i$.

## 4. Conclusions

Using the PE-FDTD simulation, the effect of the conductivity on the piezoelectric effect in PZT was investigated. The ultrasound speed and amplitude, together with the electric field, decreased with the conductivity.

## References

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