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Multiphysics Simulation of the Effect of Sensing and Spacer Layers on SAW Velocity

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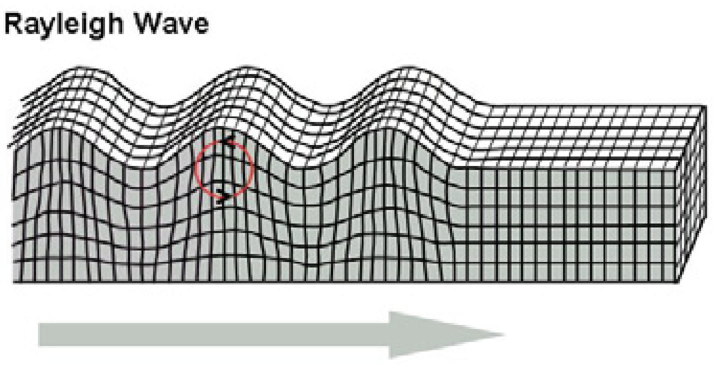
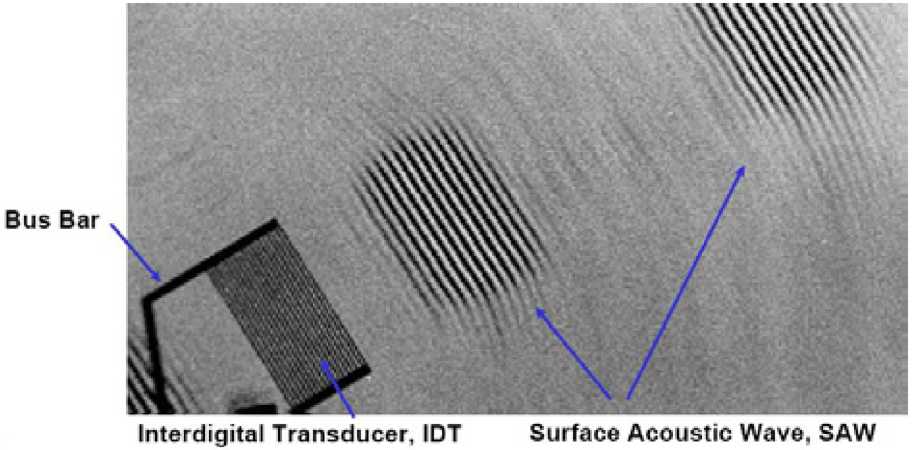
Surface Acoustic Wave (SAW) Sensor



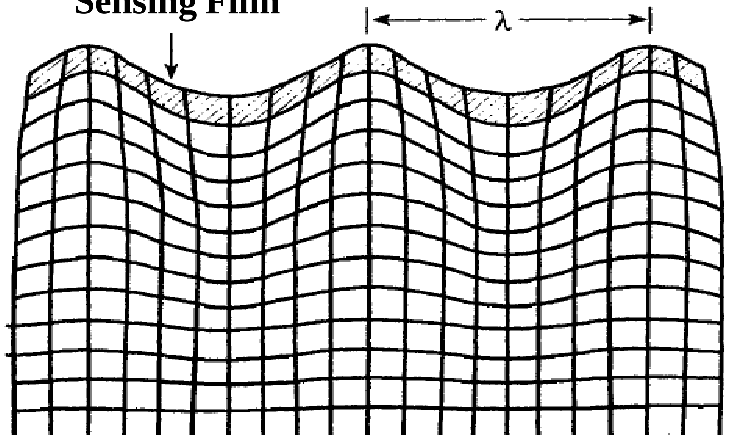
Schematic of surface acoustic wave



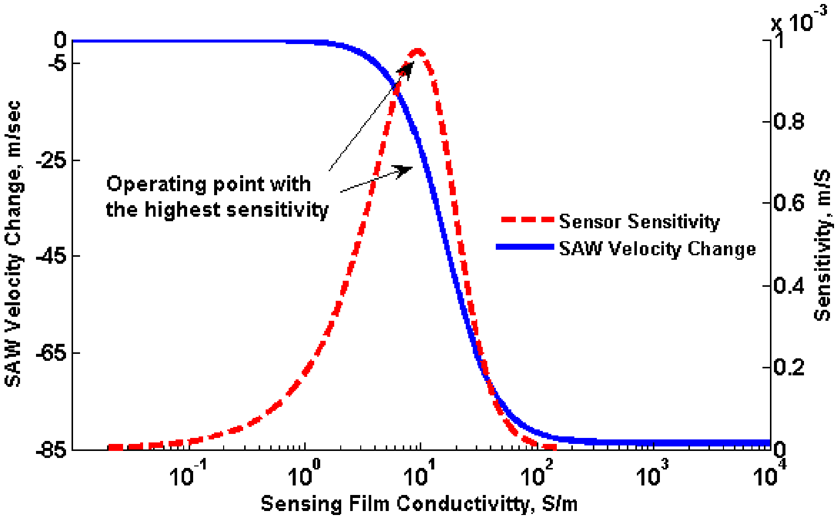
Rendl et al. UFFC 2002

- Surface acoustic wave: acoustic waves traveling along the surface of an elastic body, with an amplitude decays exponentially with depth
- SAW sensor: using interdigital transducer to detect surface acoustic wave velocity change caused by surface perturbation
  -- Surface conductivity change on piezoelectric substrate
- Research interest: SAW oxygen sensor in combustion process (up to 1000 C)

Conductivity Based SAW Gas Sensor



Acoustic Wave Sensor: Theory, Design, and Physico-Chemical Applications / Ballantine



Calculated surface acoustic wave velocity and sensitivity as a function of surface sensing film conductivity

- Conductivity based SAW gas sensor concept: A resistive gas sensing layer on piezoelectric substrate surface
- Analytic theory excludes the mechanical effect of sensing and spacer layer
- Accurate multiphysics finite element simulation is needed to include both the electrostatic effect and mechanical effect of sensing and spacer layer

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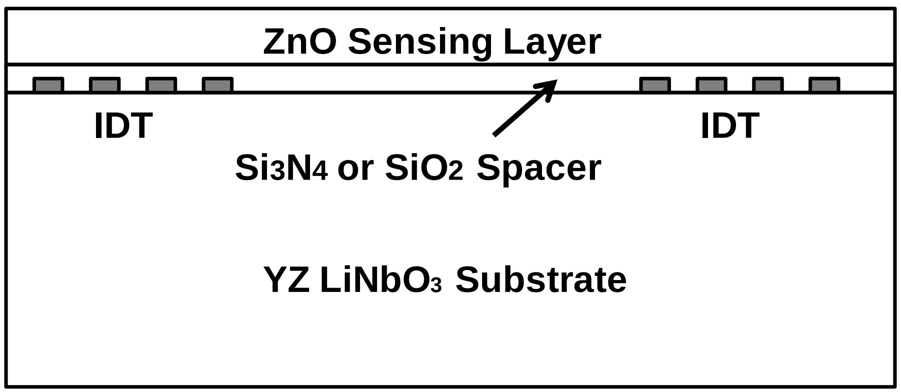
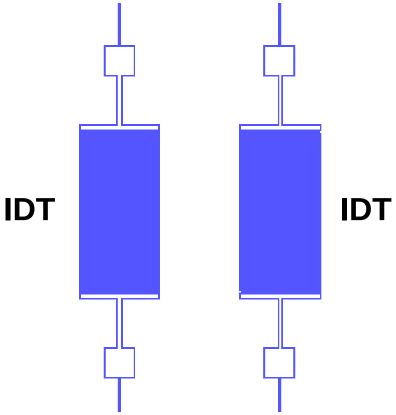
Proposed SAW Sensor Structure



Side View of SAW sensor



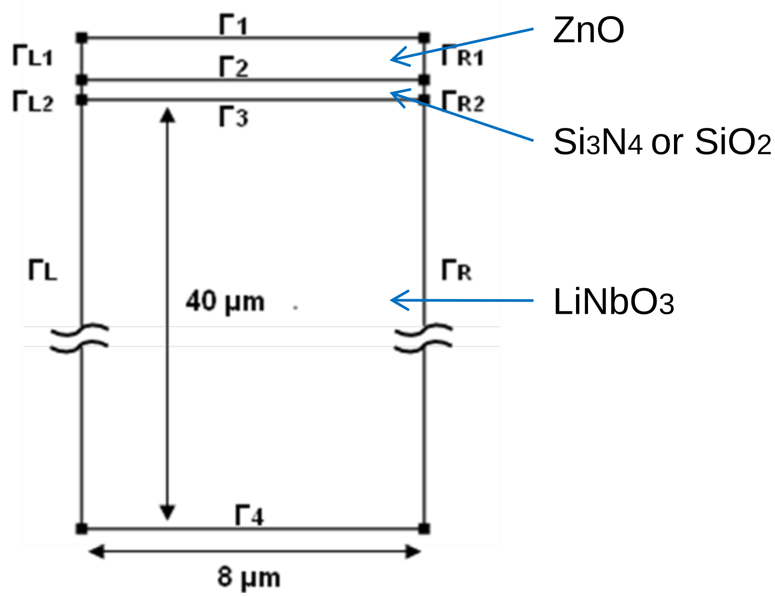
L-edit pattern of SAW sensor

- SAW gas sensor structure
  -- Oxygen surface sensing layer: ZnO;
  -- Spacer layer: Si_3N_4 or SiO_2;
  -- Piezoelectric substrate: YZ cut $LiNbO_3$;
  -- Rayleigh surface acoustic wave wavelength: λ=8 µm
- Simulation objective
  -- To analyze the effect of thickness and materials of sensing and spacer layer on sensor sensitivity
  -- To optimize the design of SAW oxygen sensor used in combustion process

Simulation Setup

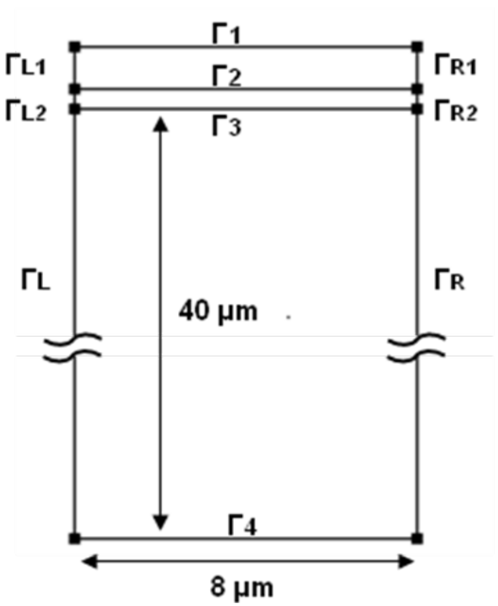
	Mechanical BC	Electrical BC
Γ_1	Free	zero charge /symmetry
Γ_{2}, Γ_2	Free	Continuity
Γ_4	Fixed	Ground
Γ_R, Γ_{R1}, Γ_{R2} Γ_L, Γ_{L1}, Γ_{L2}	Periodical boundary conditions	

Simulation Boundary Condition



- Eigenfrequency analysis in multiphysics finite element package COMSOL 3.4a 2D piezo plane strain mode (smppn)
- Periodic boundary condition to simulate the surface acoustic wave propagation
- Surface acoustic wave velocity = Eigenfrequency × Width

Simulation Setup



Continuity Equation $\nabla \cdot \vec{J} = -\frac{\partial \rho_v}{\partial t} = jw\rho_v$

Ohm's Law $\nabla \cdot \vec{J} = \nabla \cdot \sigma \vec{E} = \nabla \cdot (\sigma \varepsilon_0 \varepsilon_r \nabla V)$

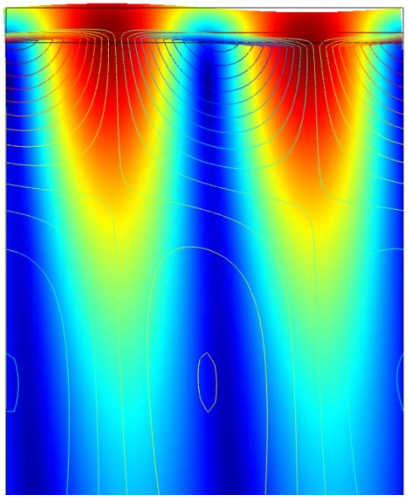
$\Rightarrow$ $\nabla \cdot (\sigma \varepsilon_0 \varepsilon_r \nabla V) = -jw\rho_v$

Electrostatic Equation $-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla V) = \rho_v$

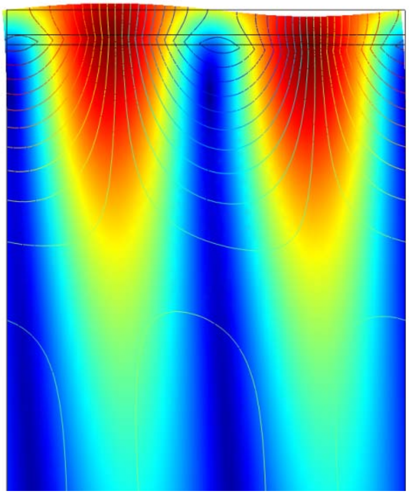
$\Rightarrow$ $-\nabla \cdot ((\frac{\sigma}{jw} + \varepsilon_0 \varepsilon_r) \nabla V) = \rho_v$

- Sensing layer: Isotropic materials mode, electric equation enabled
  -- Electrostatic equation $-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla V) = \rho_v$; Elastic equation $\mathbf{T} = c_E \mathbf{S}$
  -- Complex dielectric permittivity $\varepsilon_r - j\sigma/\omega\varepsilon_0$ to simulate conductivity
- Spacer layer: Isotropic materials mode, electric equation enabled
- Substrate: Piezoelectric materials mode
  -- Piezoelectric equation: $\mathbf{T} = c_E \mathbf{S} - e^T \mathbf{E}$ $\quad \mathbf{D} = e\mathbf{S} + \varepsilon_S \mathbf{E}$

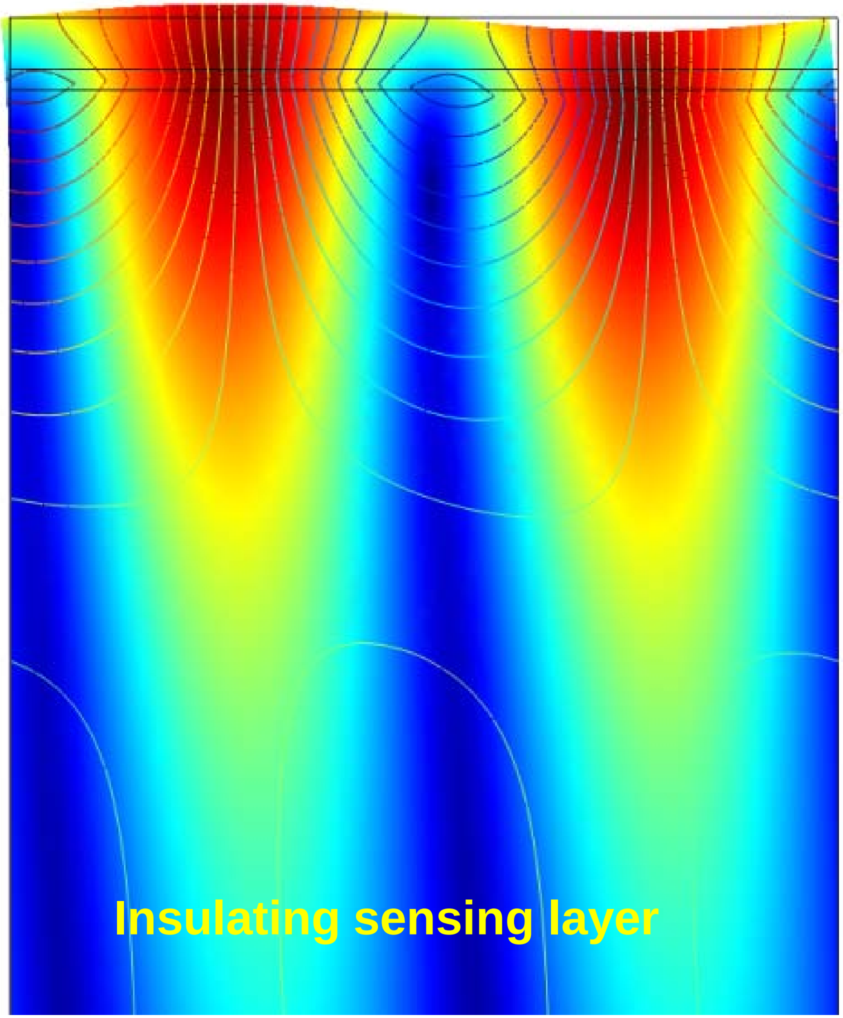
Simulation Result



Conducting sensing layer

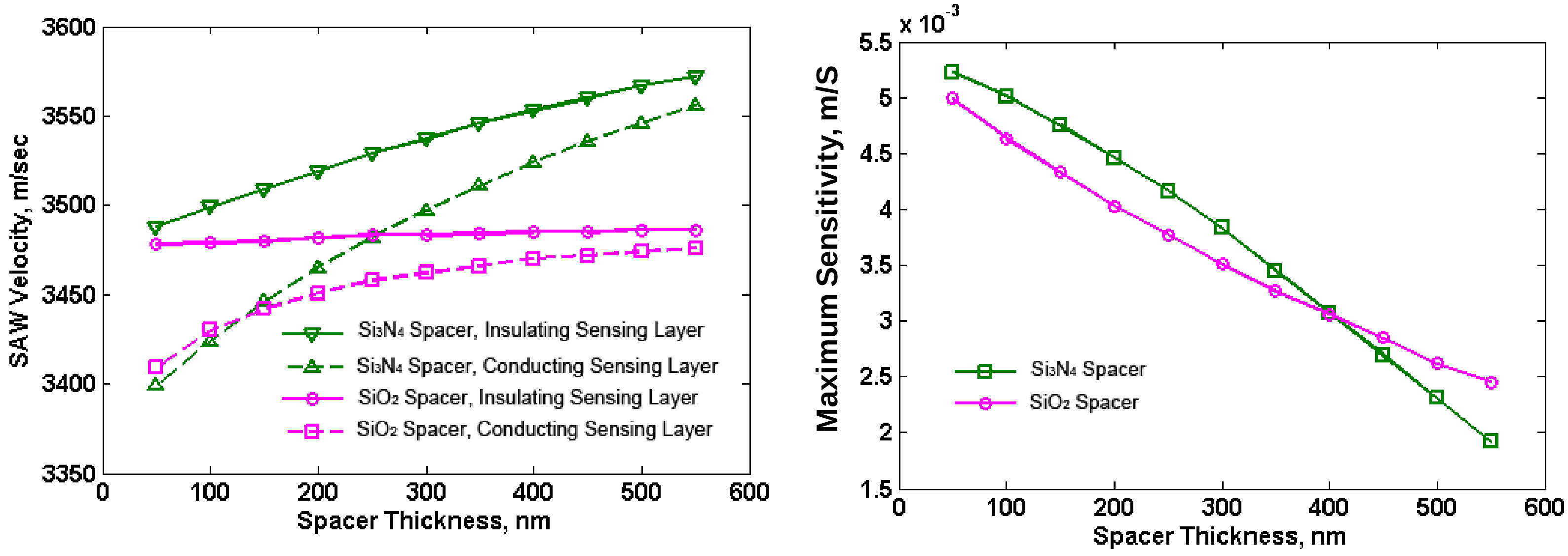


Insulating sensing layer



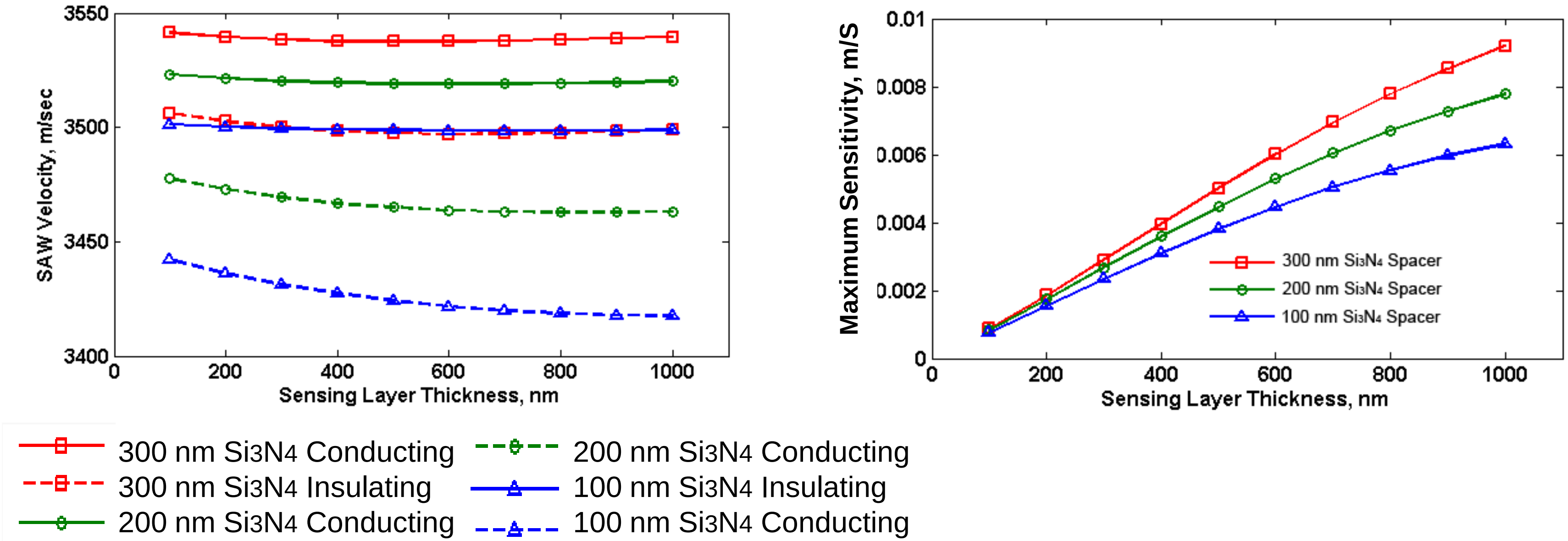
- Surface acoustic wave velocity change as a function of sensing layer bulk conductivity is simulated in different structure
- SAW sensor sensitivity is calculated by $S = -\frac{d(\Delta v / v_f)}{d\sigma_0}$

Effect of Spacing Layer



- $ZnO/Si_3N_4/LiNbO_3$ and ZnO/SiO_2 /$LiNbO_3$ structures with different spacer thickness are simulated
- $ZnO/Si_3N_4/LiNbO_3$ structure has better sensitivity than ZnO/SiO_2 /$LiNbO_3$ when the spacer is thinner than 400 nm
- The $ZnO/Si_3N_4/LiNbO_3$ structure is selected for the following simulation

Effect of Sensing Layer



- $ZnO/Si_3N_4/LiNbO_3$ structure with different sensing layer thickness are simulated
- The maximum sensitivity increase linearly as sensing layer thickness increase
- Thicker sensing layer has larger film conductivity change $\sigma_{film} = \sigma_{bulk} t$ resulting a higher sensitivity

Summary

- Surface acoustic wave propagation in $ZnO/Si_3N_4/LiNbO_3$ and $ZnO/SiO_2/LiNbO_3$ layered structures are simulated using COMSOL 3.4a 2D piezo plane strain mode.
- The effect of thickness and materials of sensing and spacer layer on the sensitivity are analyzed to optimize SAW gas sensor design
- The simulation result shows that the maximum sensitivity increase as the spacer gets thinner or the sensing layer gets thicker for both layered structure
- $ZnO/Si_3N_4/LiNbO_3$ layered structure shows higher sensitivity than the $ZnO/SiO_2/LiNbO_3$ layered structure with a spacer thickness ranges from 50 nm to 400 nm