Non-uniform and anisotropic dielectric constant of ultrathin Si(001)

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2019/06/26

Motivation

- **Dielectric constant**

$$\varepsilon = \varepsilon_0 \varepsilon_r = \varepsilon_0 \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix}$$

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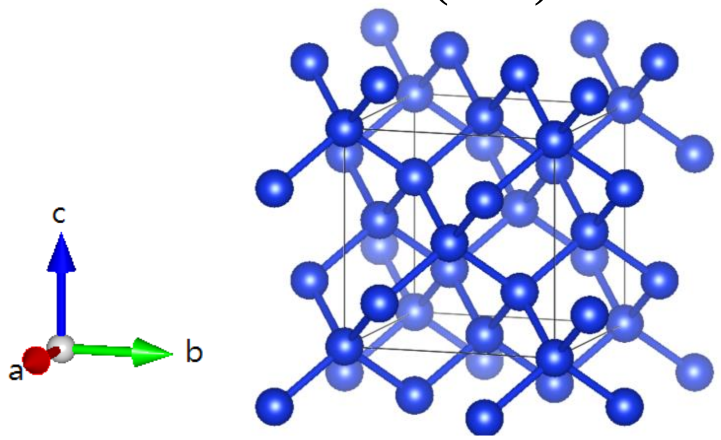
homogeneous and isotropic

Si ($\varepsilon_r \approx 12$)

$$\varepsilon = \varepsilon_0 \varepsilon_r = \varepsilon_0 \varepsilon_r \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Cubic diamond lattice structure
(bulk)



Motivation

- **Dielectric constant**

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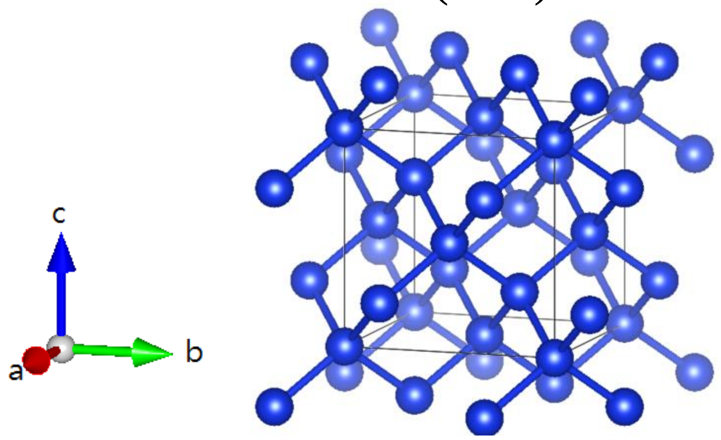
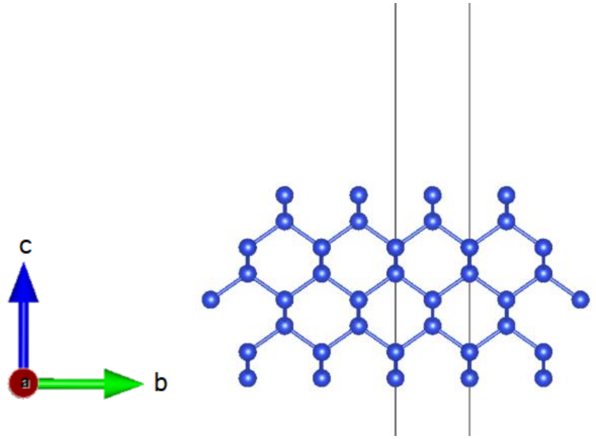


Ultrathin slab



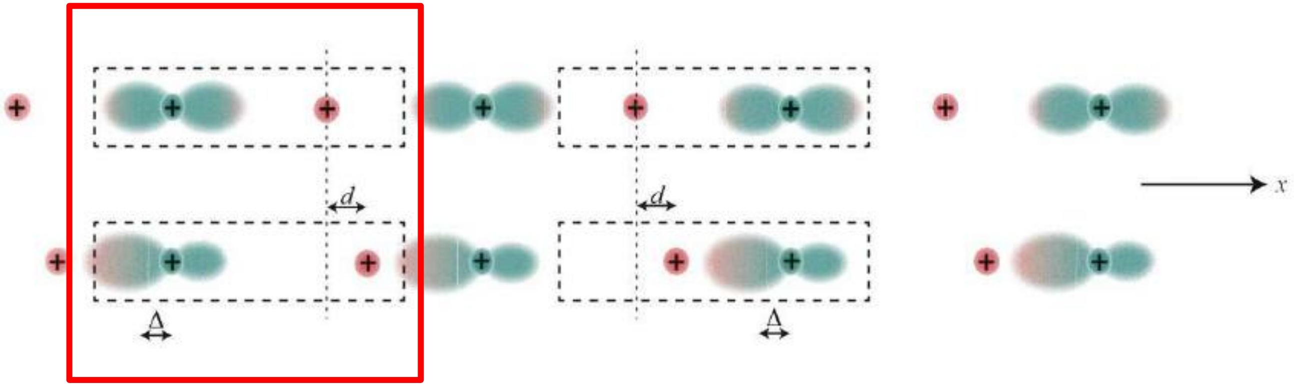
$\varepsilon_r = \varepsilon_{xx} (= \varepsilon_{yy}) = \varepsilon_{zz}$?

Methodology

- **Modern theory of polarization : a well definition in periodic solid**

Initial state

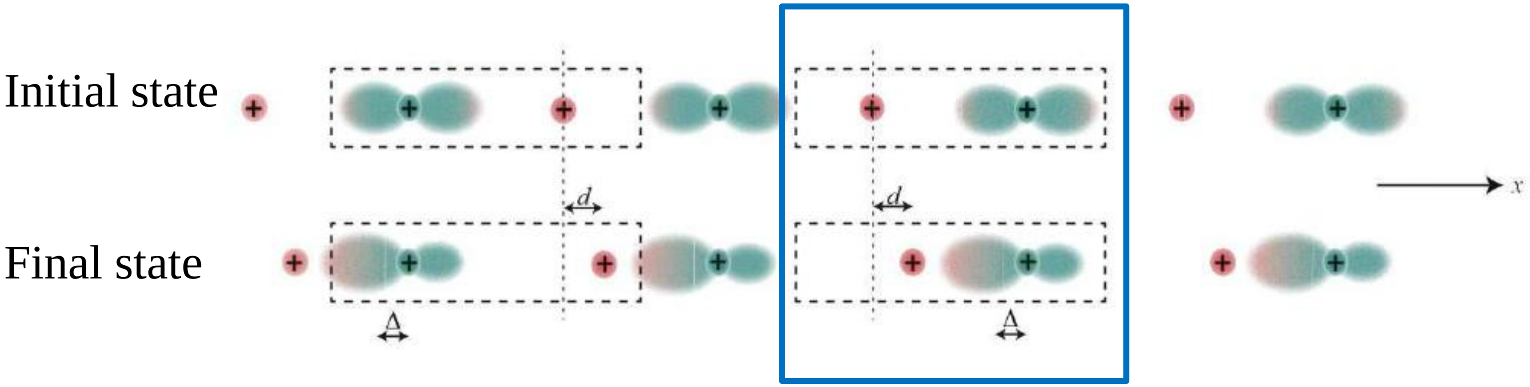
Final state



	Red cell	Blue cell
Initial state	$+\frac{1}{2}$	
Final state	$+\frac{1}{2}+dip$	

Methodology

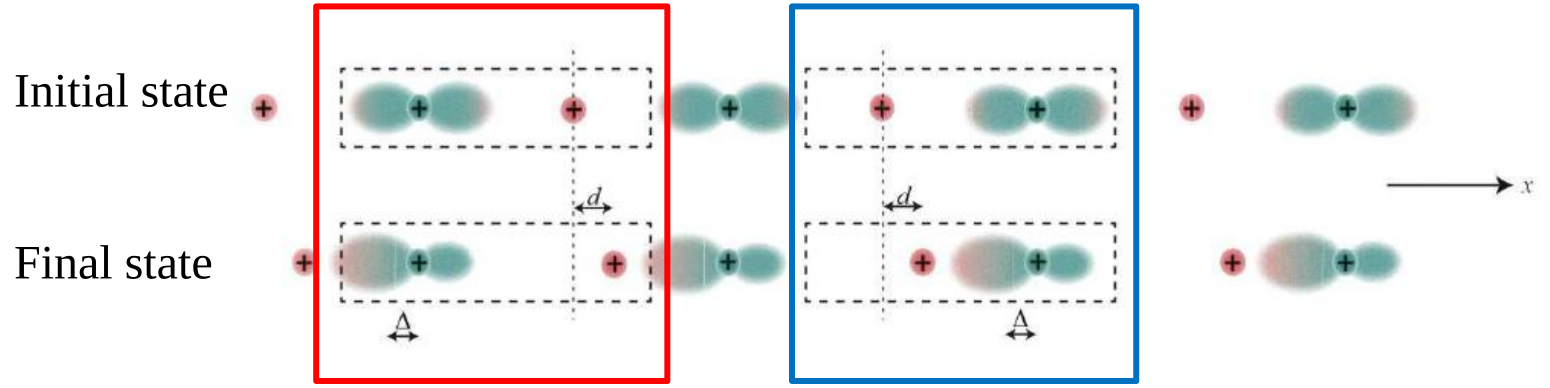
➢ **Modern theory of polarization : a well definition in periodic solid**



	Red cell	**Blue cell**
Initial state		$-\frac{1}{2}$
Final state		$-\frac{1}{2}-dip$

Methodology

➢ **Modern theory of polarization : a well definition in periodic solid**



	Red cell	Blue cell
Initial state	$+\frac{1}{2}$	$-\frac{1}{2}$
Final state	$+\frac{1}{2}+dip$	$-\frac{1}{2}-dip$
***dip* = $2\Delta + d$ (well definition)**		

The polarization of each state is a relative property.

$$\Delta \mathbf{P}_e = \mathbf{P}_e^{(\lambda_2)} - \mathbf{P}_e^{(\lambda_1)}$$

The change in polarization is well definition in periodic solid.

$$\varepsilon_{ij} - \delta_{ij} = \frac{4\pi}{\varepsilon_0}\frac{\partial P_i}{\partial E_j}; \mathrm{i,j = x,y,z}$$

Methodology

- **Modern theory of polarization: berry phase method**

$$\mathbf{P}_e^{(\lambda)} = -\frac{if|e|}{8\pi^3}\sum_{n=1}^{M}\int_{BZ} d^3k \langle u_{n\mathbf{k}}^{(\lambda)}|\nabla_{\mathbf{k}}|u_{n\mathbf{k}}^{(\lambda)}\rangle$$

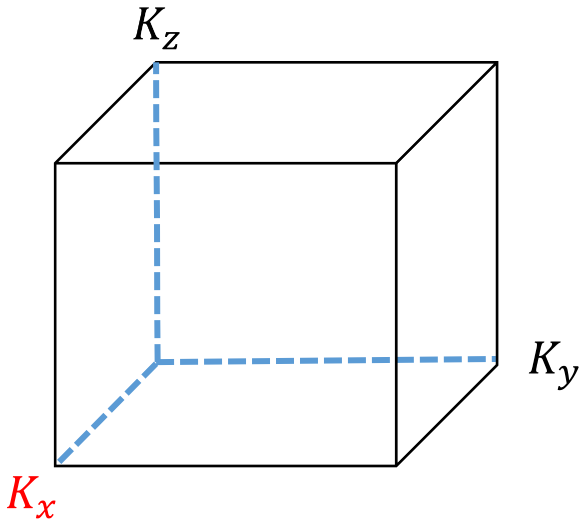
R. D. King-Smith and D. Vanderbilt, Phys. Rev. B 47, 1651 (1993).

Methodology

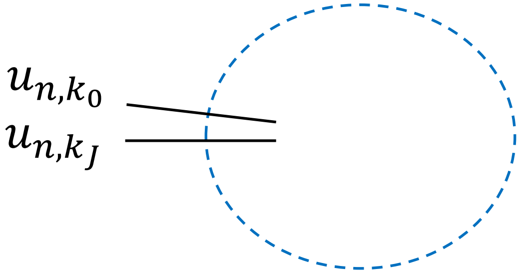
- **Modern theory of polarization: berry phase method**

$$\mathbf{P}_e^{(\lambda)} = -\frac{if|e|}{8\pi^3}\sum_{n=1}^{M}\int_{BZ} d^3k \langle u_{n\mathbf{k}}^{(\lambda)} | \nabla_{\mathbf{k}} | u_{n\mathbf{k}}^{(\lambda)} \rangle$$

IBZ



"J" cuts



Eigenstate: u_{n,k_j}

$n = (valence) band\ index$

k_j = # of cut point

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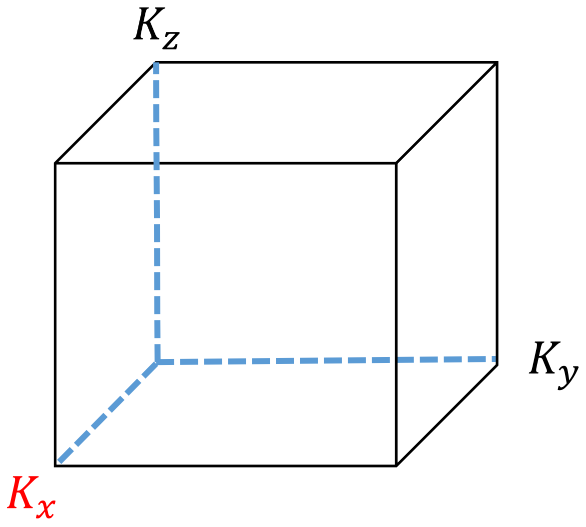

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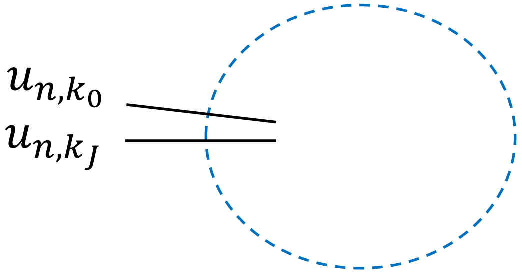


Eigenstate: u_{n,k_j}

$n = (valence)band\ index$

k_j = # of cut point

$$u_{n,k_0}(r) = e^{-iG\cdot r}\, u_{n,k_J}(r)$$

$$\phi_J^{(\lambda)}(\mathbf{k}_\perp) = \mathrm{Im}\left\{\ln \prod_{j=0}^{J-1} \det\left(\langle u_{m\mathbf{k}_j}^{(\lambda)}|u_{n\mathbf{k}_{j+1}}^{(\lambda)}\rangle\right)\right\}$$

position of electron clouds center in 2π unit.

$$(\boldsymbol{P}_e)_i = \frac{f|e|R_i}{2\pi\Omega_0}\phi_J$$

R. D. King-Smith and D. Vanderbilt, Phys. Rev. B 47, 1651 (1993).

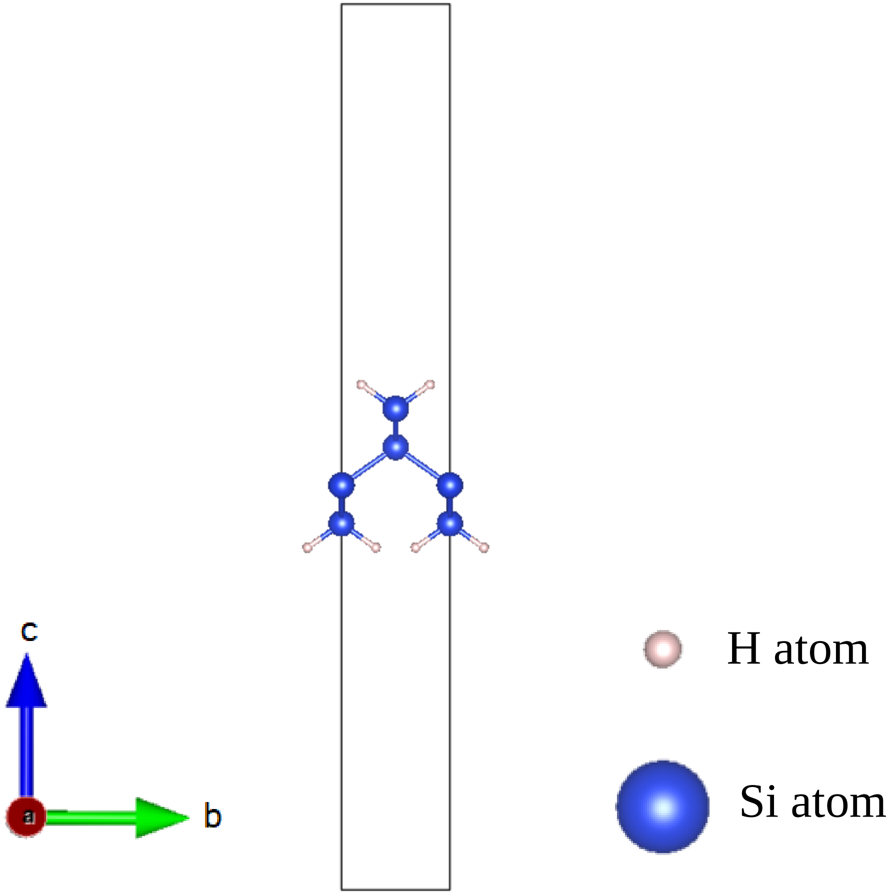
Methodology

- **Tool: VASP 5.4.4**

- Generalized gradient approximation(GGA) of the Perdew-Burke-Enzerhof (PBE) form.
- The plane wave cutoff energy is taken as 500 eV.
- 13×13×13 for bulk(13×13×1 for slab) Gamma-centered k-mesh.

Methodology

➢ **The structure of slab**

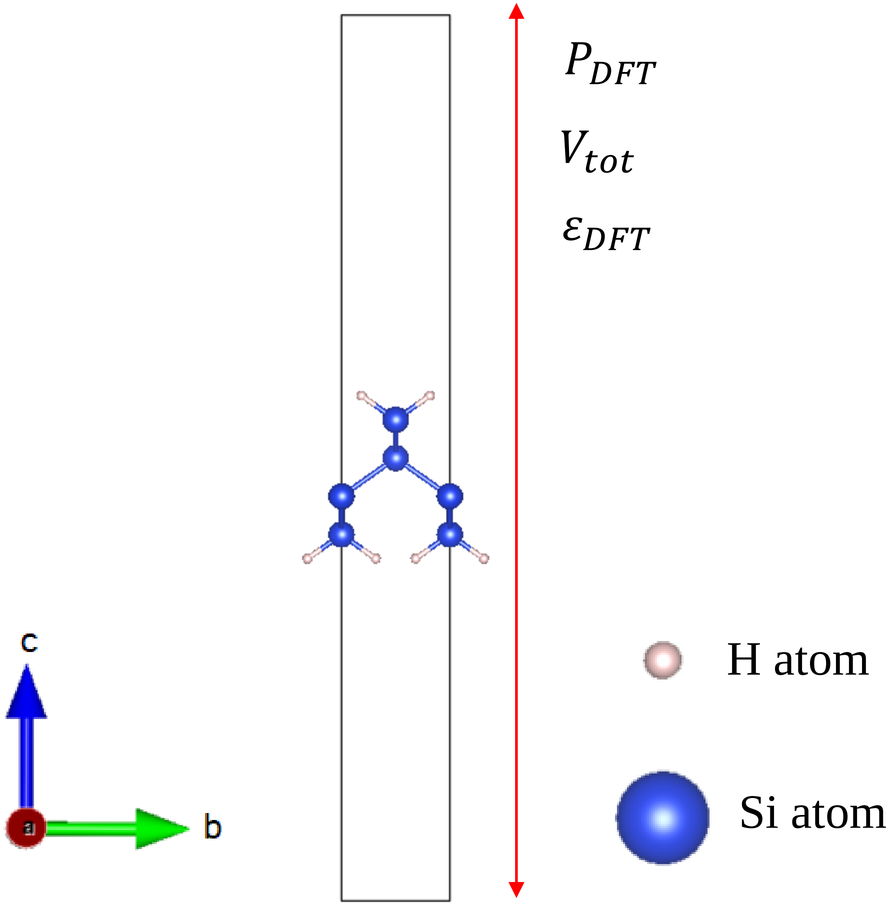


➢ Si-H: Eliminate the dangling bond.

➢ Vacuum: avoid interaction.

Results and discussions

- **The result of dielectric constant from DFT by using berry phase method**



$$\varepsilon_{DFT} - 1 = \frac{4\pi}{\varepsilon_0}\frac{\partial P}{\partial E}$$

Results and discussions

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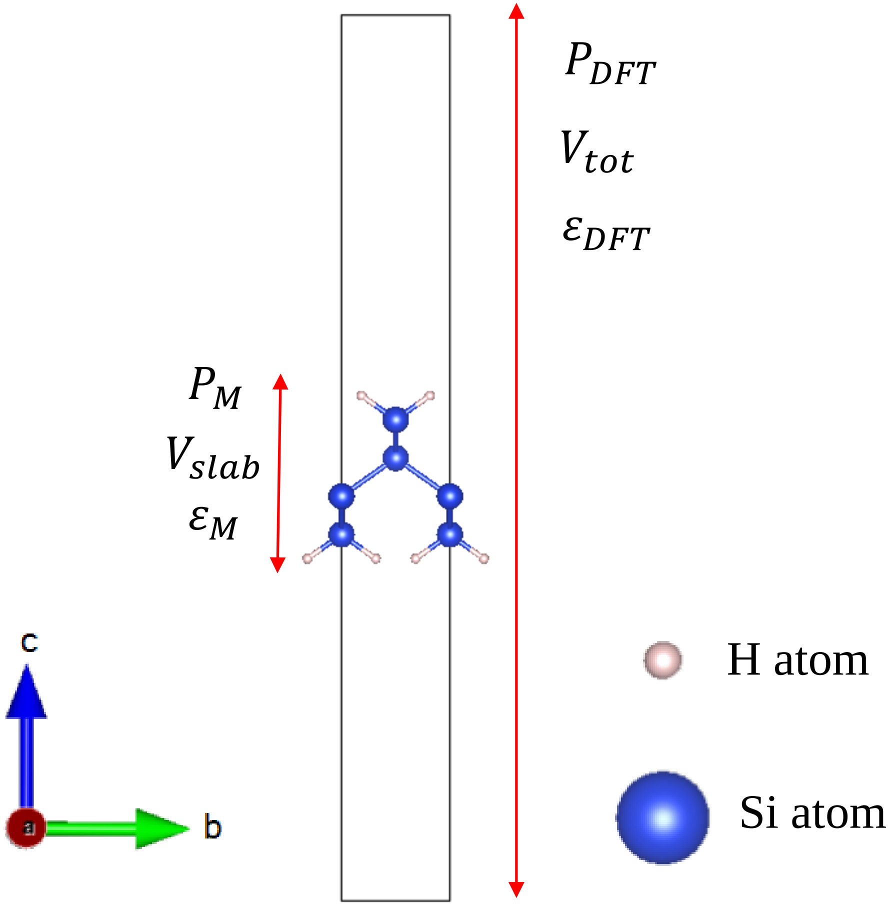


$$\varepsilon_{DFT} - 1 = \frac{4\pi}{\varepsilon_0}\frac{\partial P}{\partial E}$$

$$P_{DFT} = \frac{V_{tot}}{V_{slab}} \times P_M;$$ (no contribution from vacuum)

Fitting function:

$$(\varepsilon_{DFT} - 1) = \frac{P_{DFT}}{P_M} \times (\boldsymbol{\varepsilon_M} - 1)$$

$$= \frac{\varepsilon_M - 1}{1 + \frac{V_{vacuum}}{V_{slab}}};$$

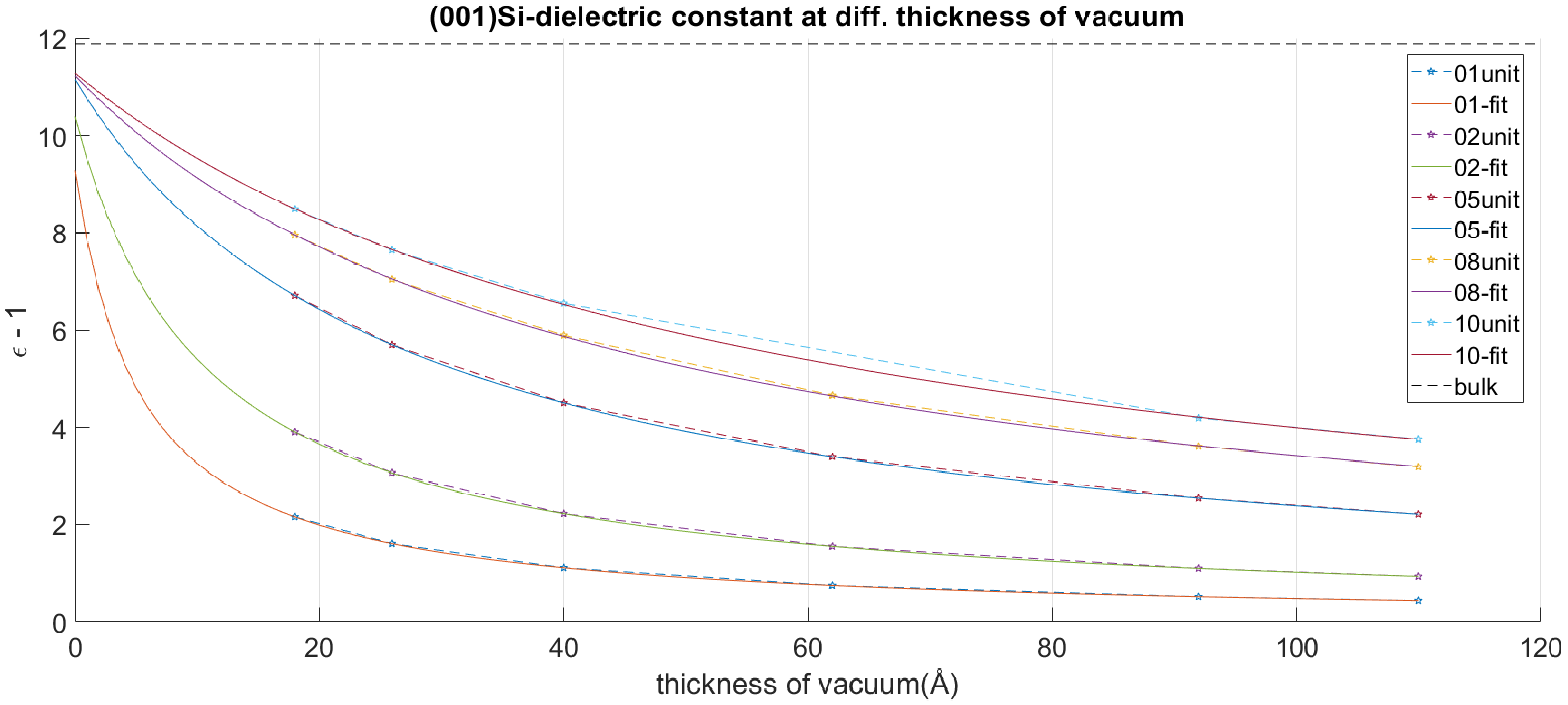
This is what we need.

Results and discussions

- **The result of dielectric constant $\varepsilon_{xx,yy}$**

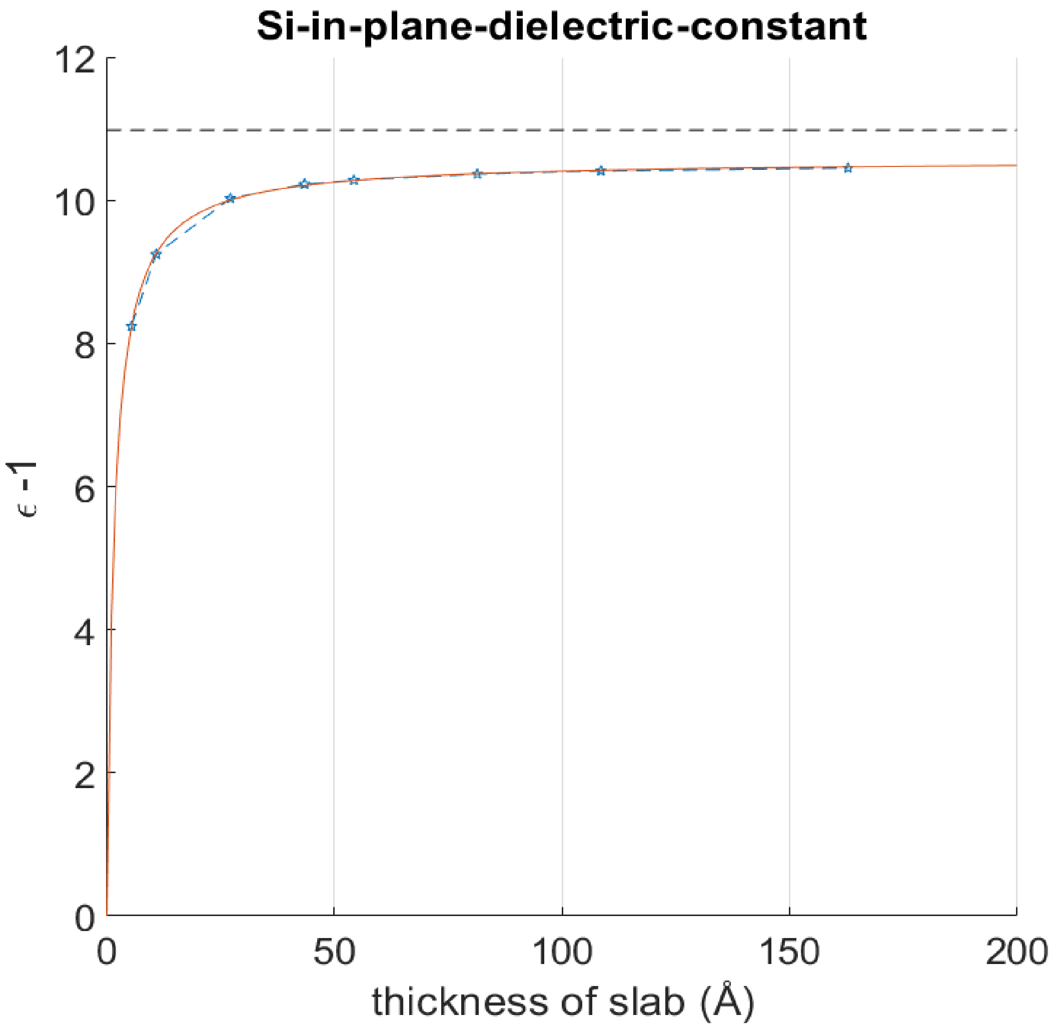
Fitting function:

$$(\varepsilon_{DFT} - 1) = \frac{\varepsilon_M - 1}{1 + \frac{V_{vacuum}}{V_{slab}}};$$



Results and discussions

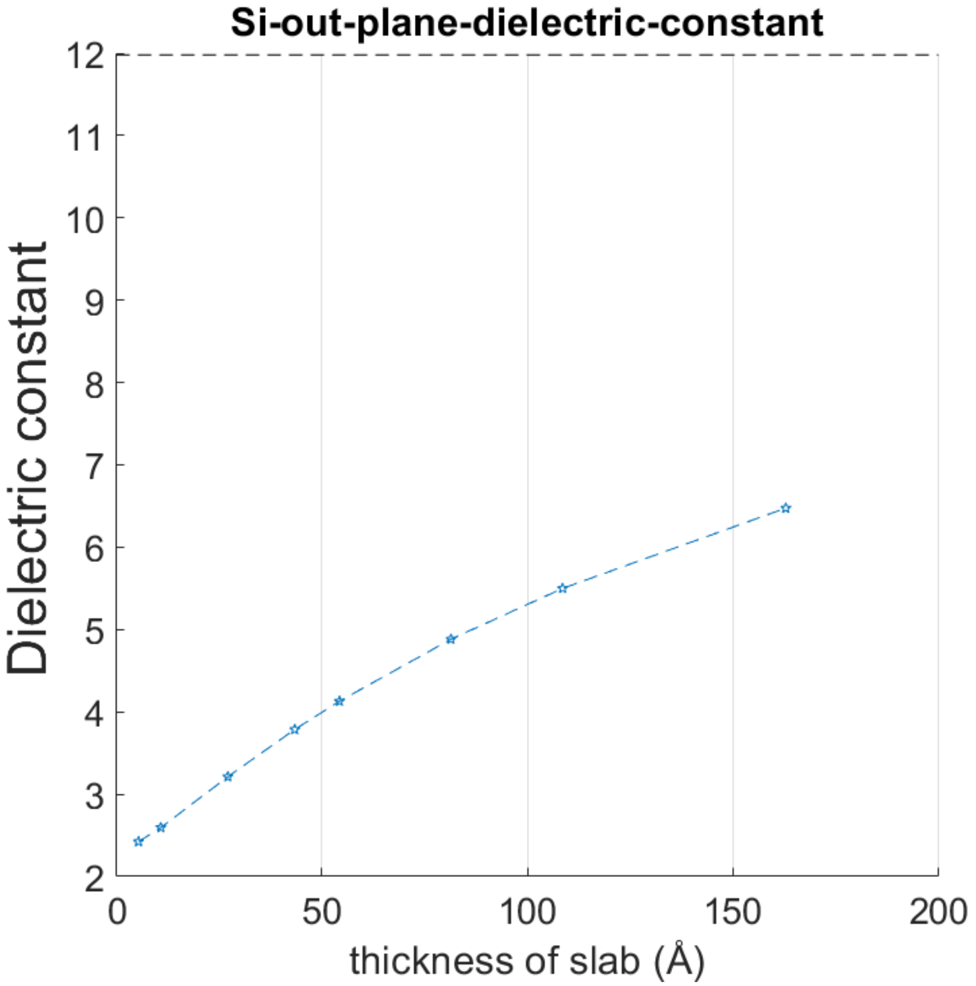
- **The result of dielectric constant $\varepsilon_{xx,yy}$**



- Saturation around 50Å of thickness.
- Decrease with thinner thickness.

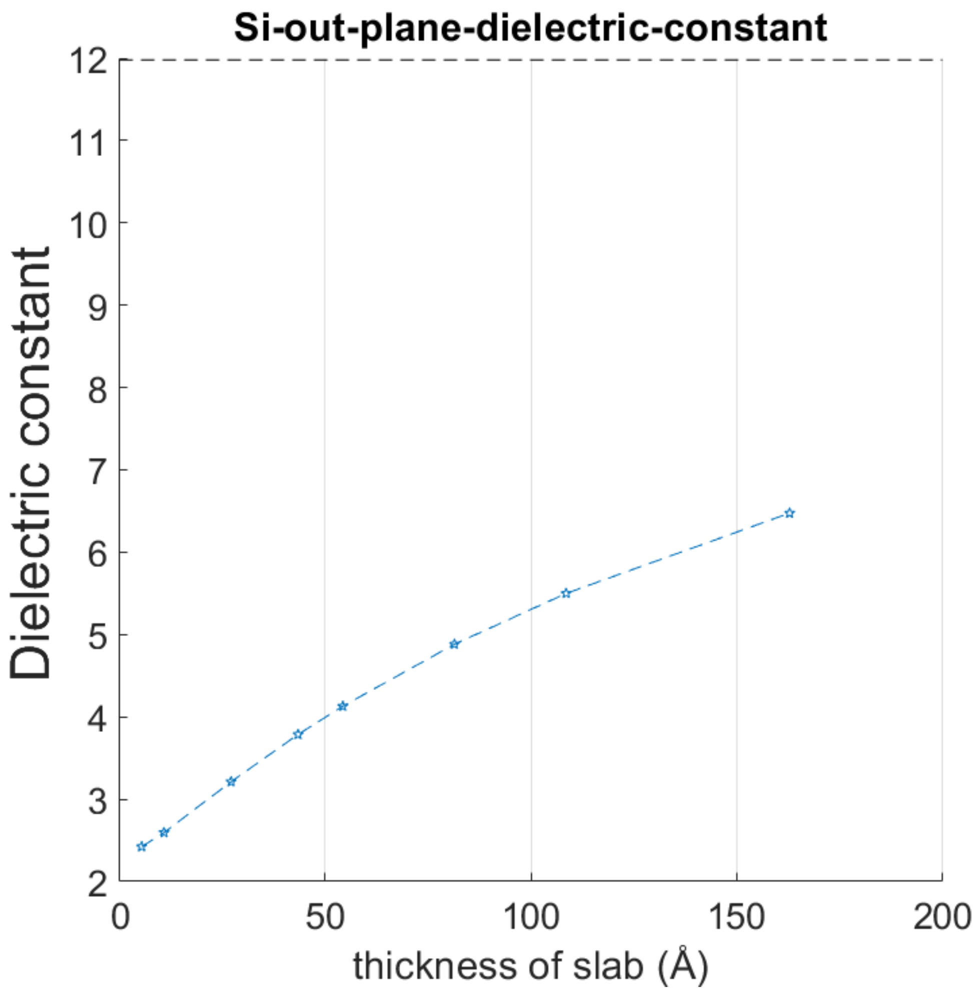
Results and discussions

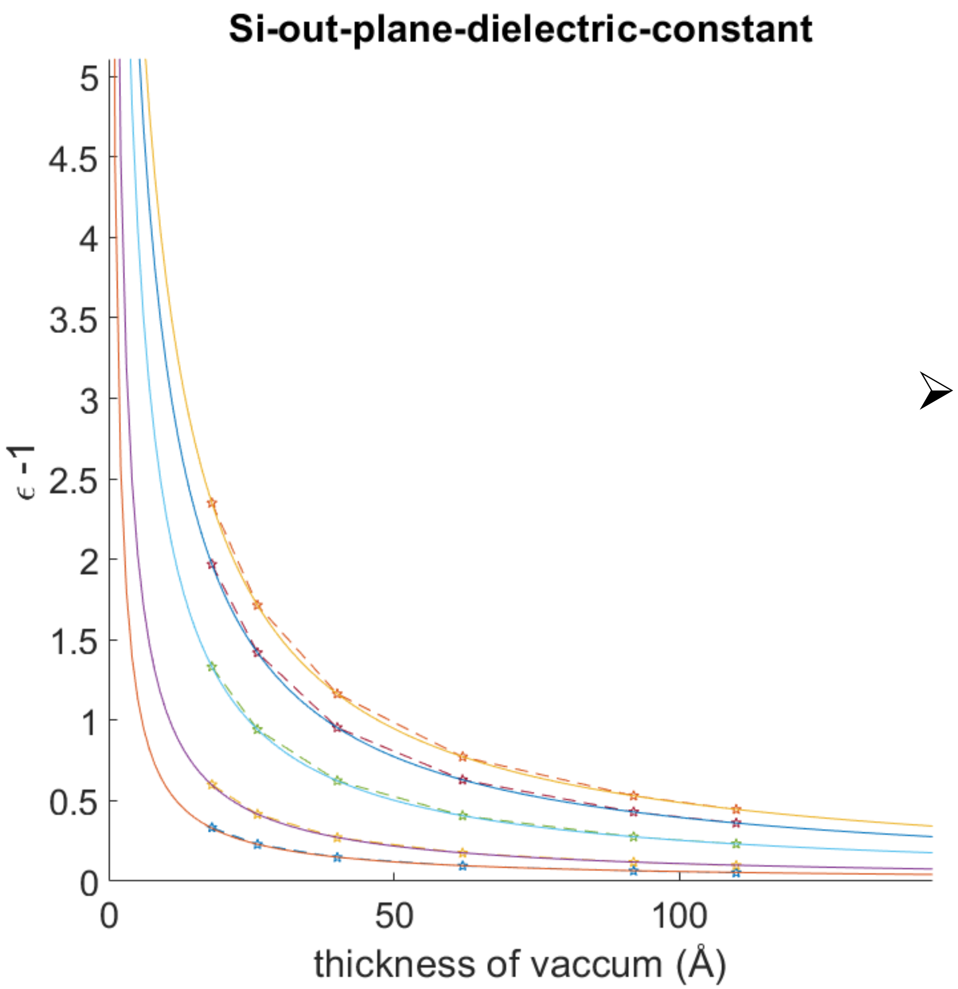
- **The result of dielectric constant ε_{zz}**



Results and discussions

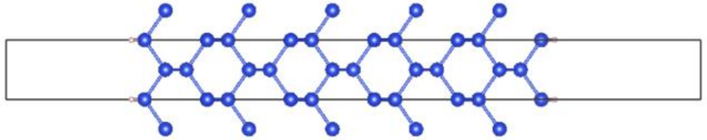
- The result of dielectric constant ε_{zz}



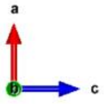


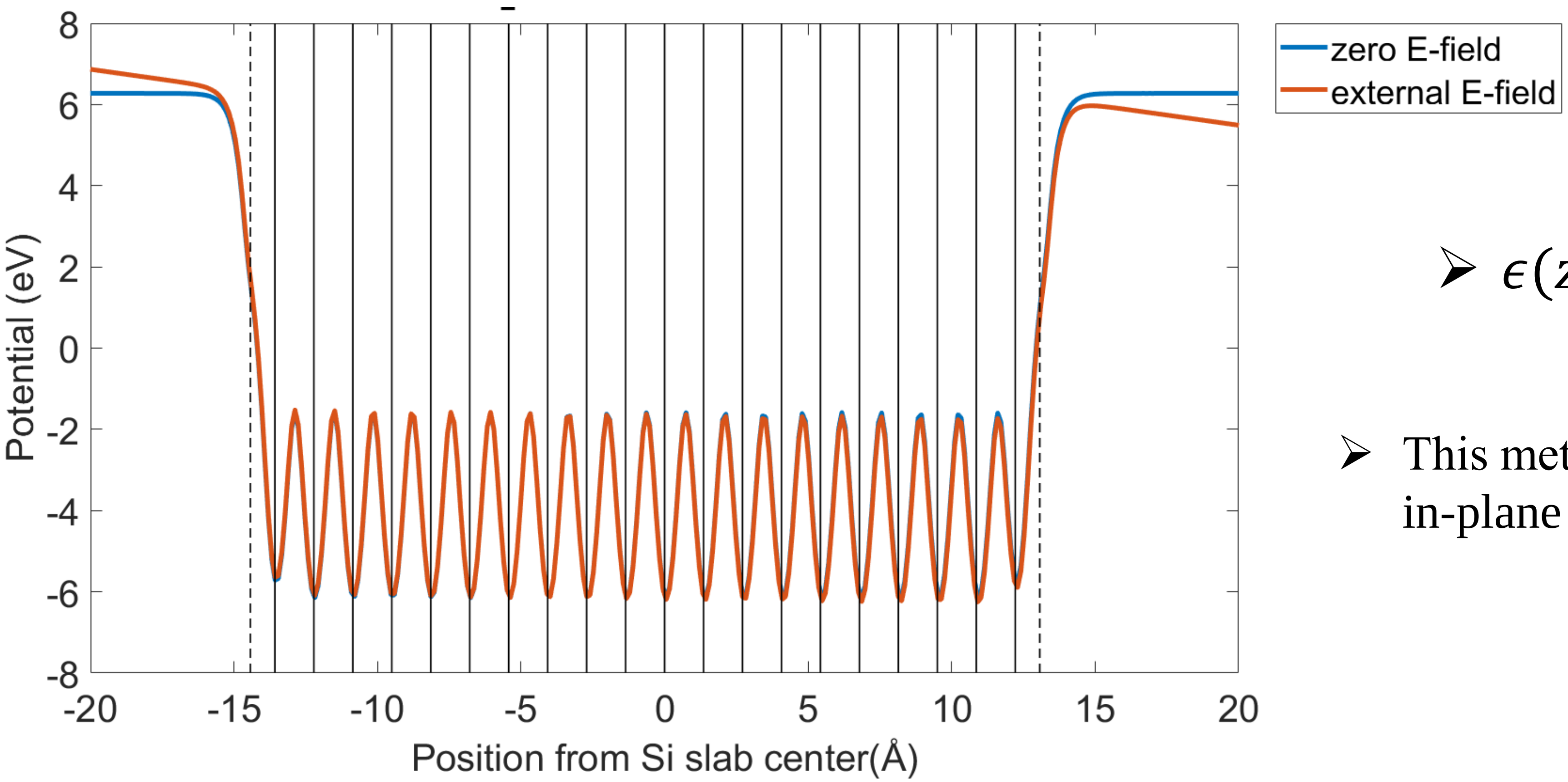
- $P_{DFT} \neq \frac{V_{tot}}{V_{slab}} \times P_M$?

Results and discussions



- **The result of dielectric constant ε_{zz}**



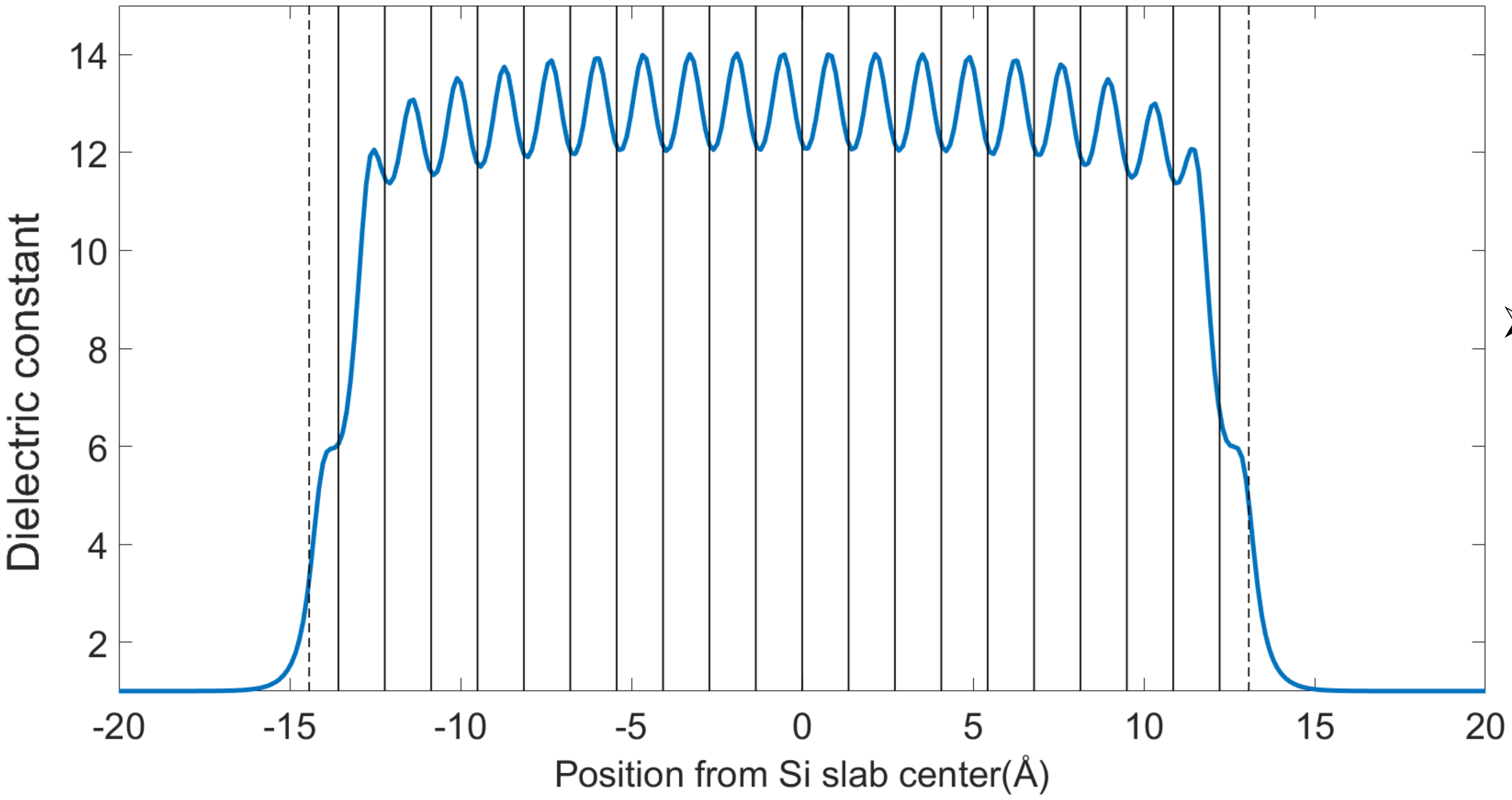


- $\epsilon(z) = \frac{E_{in}}{E_{ext}} = \frac{\frac{\partial \Delta V_{in}(z)}{\partial z}}{E_{ext}}$

- This method doesn't be used along in-plane direction.

Results and discussions

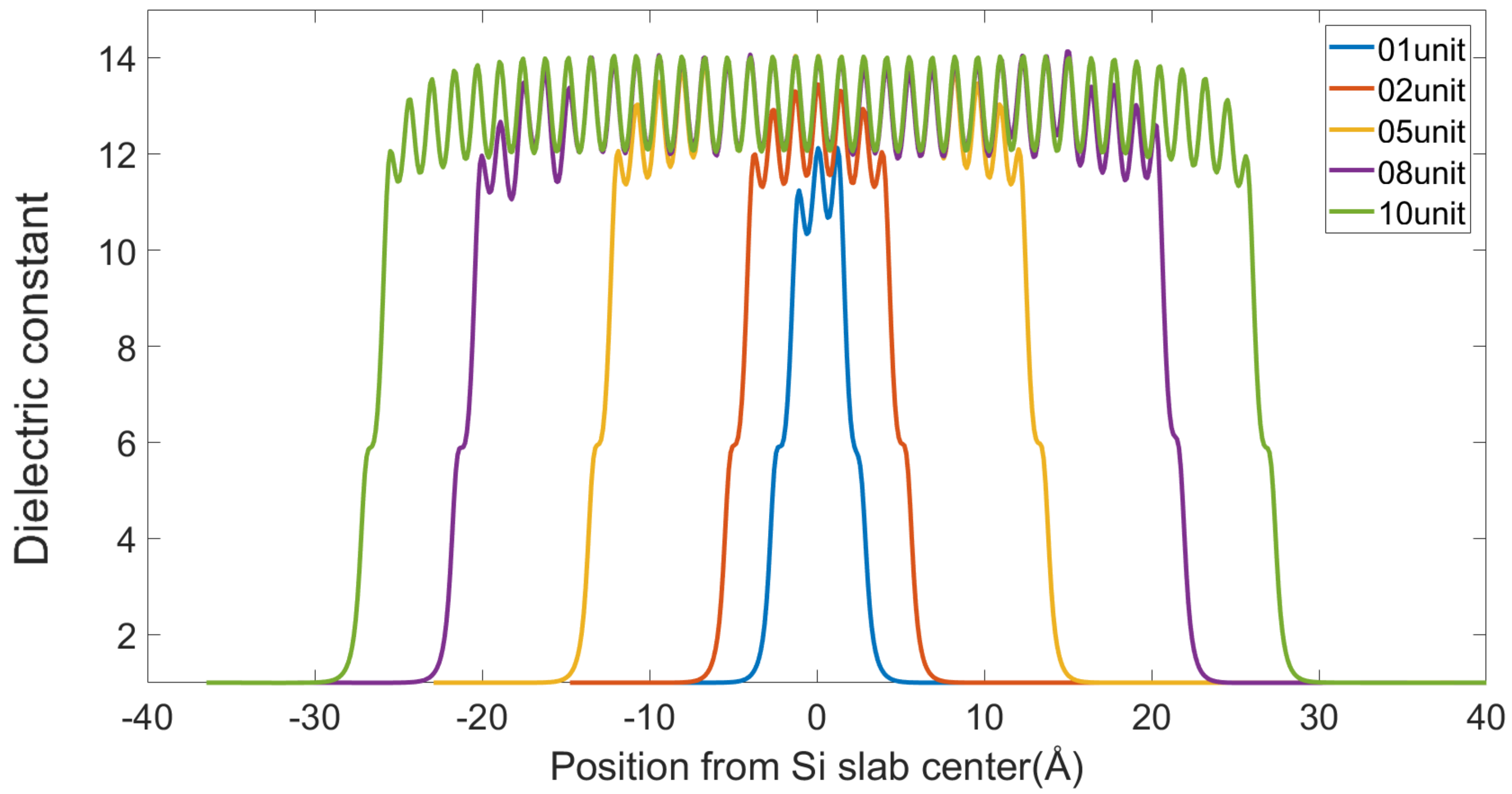
- **The result of dielectric constant ε_{zz}**



- The dielectric constant function of z.

Results and discussions

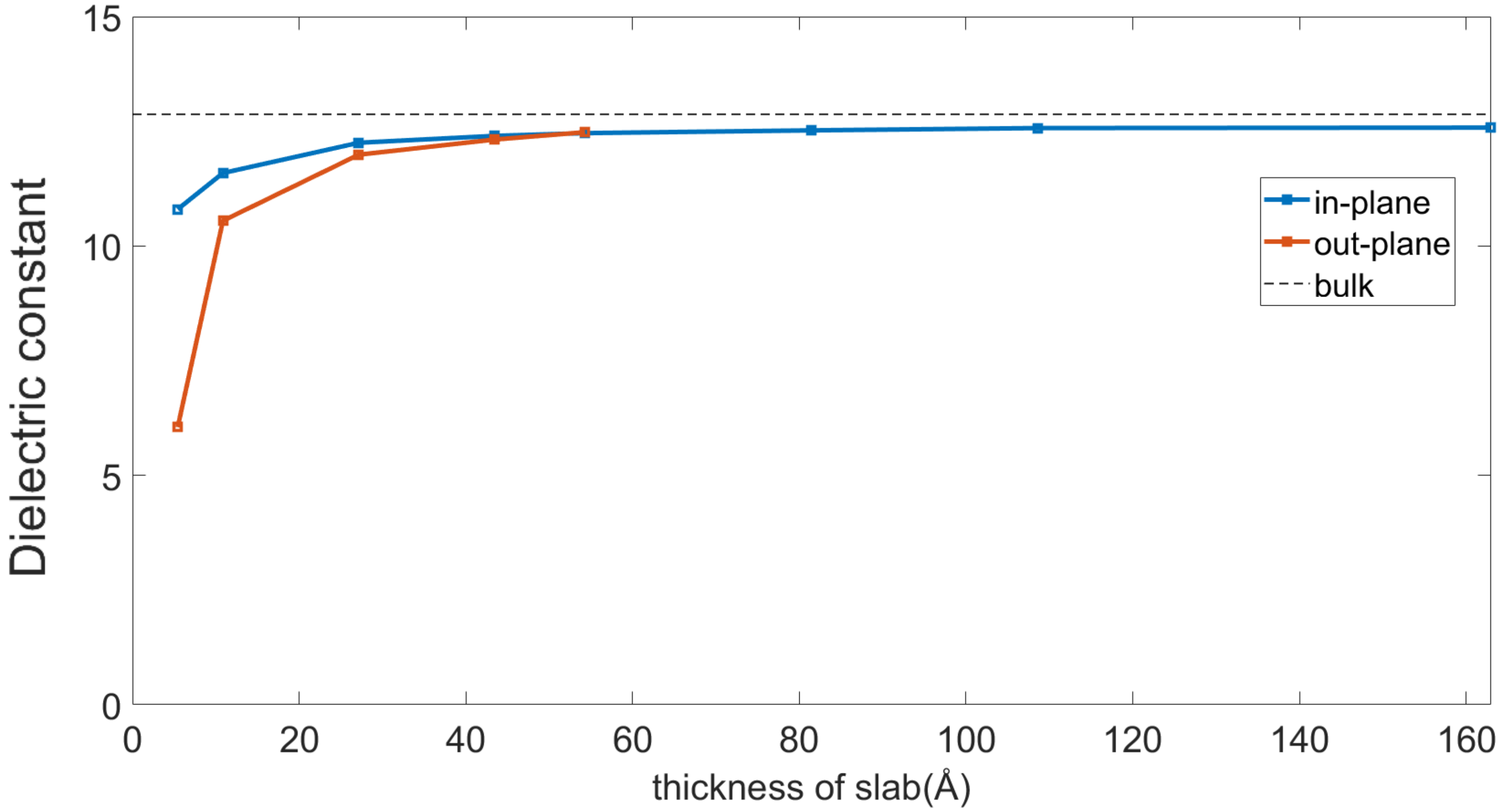
- **The result of dielectric constant ε_{zz}**



- ε_{zz}(z) is non-uniform.
- <ε_{zz}> decays as thickness of slab decreases.

Results and discussions

- **The result of dielectric constant $\varepsilon_{xx}, \varepsilon_{yy}$, ε_{zz}**



- Anisotropy in ultrathin Si(001).
  - $\varepsilon_{xx} = \varepsilon_{yy} \neq \varepsilon_{zz}$
- Isotropy in Si if the thickness is larger than 50Å .

Summary

- The property of dielectric constant ε_{zz}(z) in edge is smaller than center.
- The average dielectric constant $\varepsilon_{xx}(\varepsilon_{yy})$, $<\varepsilon_{zz}>$ decays as thickness of slab decreases.
- The dielectric constant $\varepsilon_{xx}(\varepsilon_{yy}), \varepsilon_{zz}$ is anisotropy in ultrathin Si(001).
- When the thickness of Si is larger than 50 Å , the dielectric constant is isotropy and close to bulk.

Summary

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 66, NO. 6, JUNE 2019 2509

Impact of Semiconductor Permittivity Reduction on Electrical Characteristics of Nanoscale MOSFETs

Si-Hua Chen, Shang-Wei Lian, Tzung Rang Wu, Tay-Rong Chang, Jia-Ming Liou, Darsen D. Lu, Kuo-Hsing Kao, *Member, IEEE*, Nan-Yow Chen, Wen-Jay Lee, and Jyun-Hwei Tsai

Thanks for listening