ACM 114 Presentation – 05/02/2012

Parallel Implementation of Phase field Modeling of Ferroelectric Domain formation

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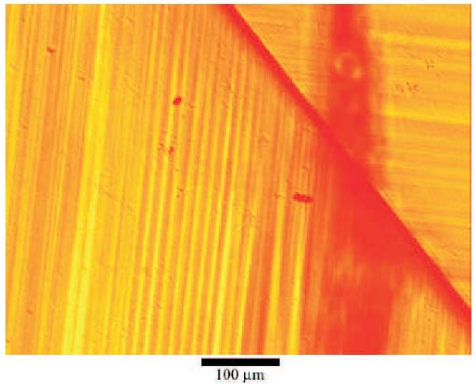
ME Option



Domain wall as seen in an experiment

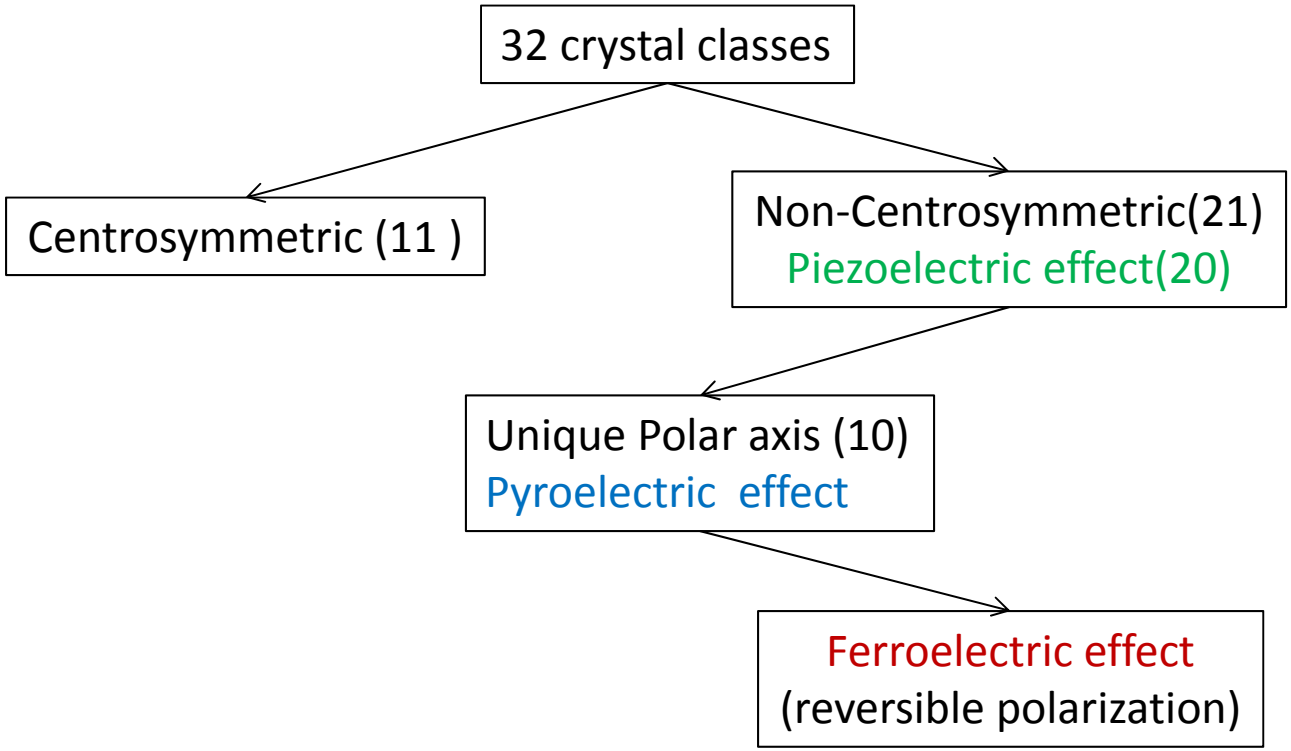
(Burcsu, 2001)

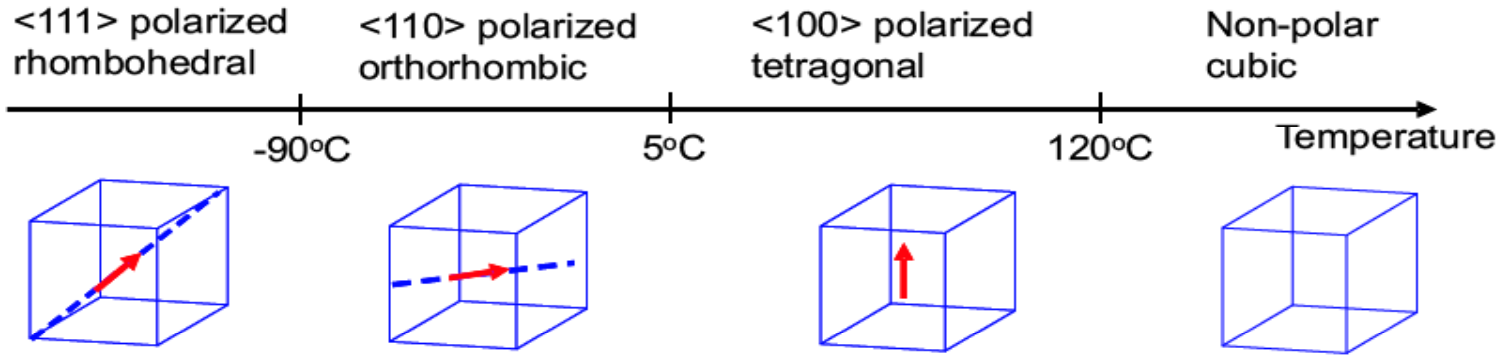
Ferroelectric crystals

- A ferroelectric crystal is non-polar (paraelectric) above its Curie temperature, but is spontaneously polarized (ferroelectric) below the Curie temperature.

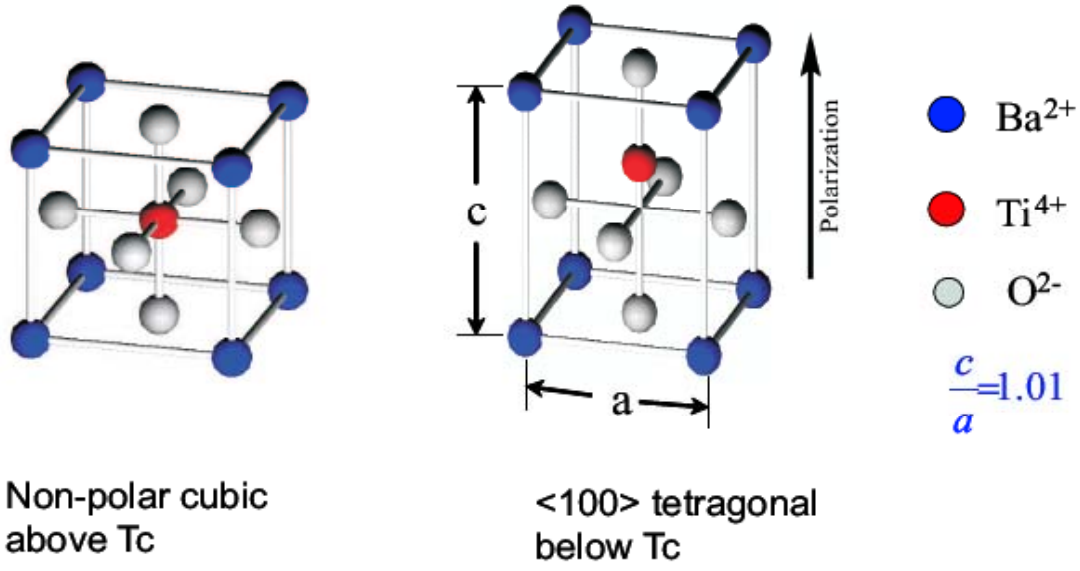
- The spontaneous polarization can be switched through the application of an electric field or mechanical stress.

Examples: Rochelle salt $(NaKC_4H_4O_6.4H_2O)$; KH_2PO_4 ; $BaTiO_3$; $NaNO_2$





Various crystalline phases of $BaTiO_3$.



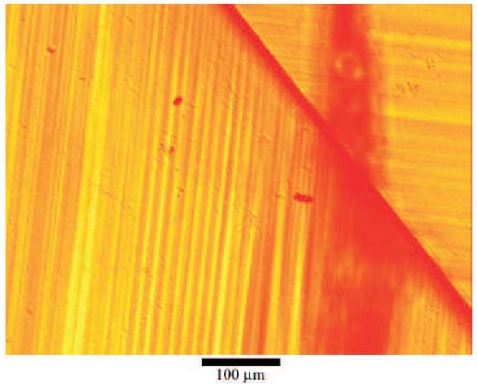
Crystal structures of $BaTiO_3$ in their cubic and tetragonal phases.

Domains of variants

- A reduction of crystal symmetry at Curie temperature gives rise to symmetry-related ***variants*** (crystallographically and energetically identical states that are oriented differently with respect to the parent non-poplar state).

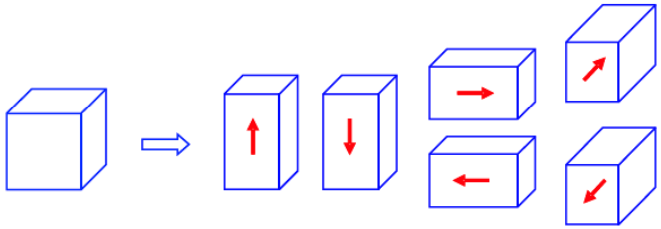
- Variants can coexist as domains separated by domain walls.

- Variants are *energy-equivalent* ⟹ It is possible to switch one domain to another by suitable electromechanical loading.

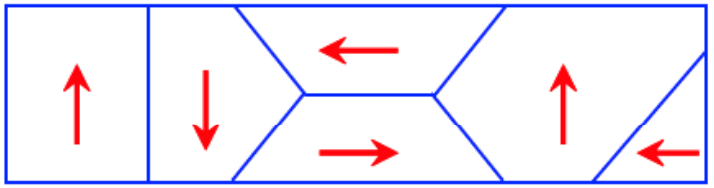


Domain wall as seen in an experiment

(Burcsu, 2001)

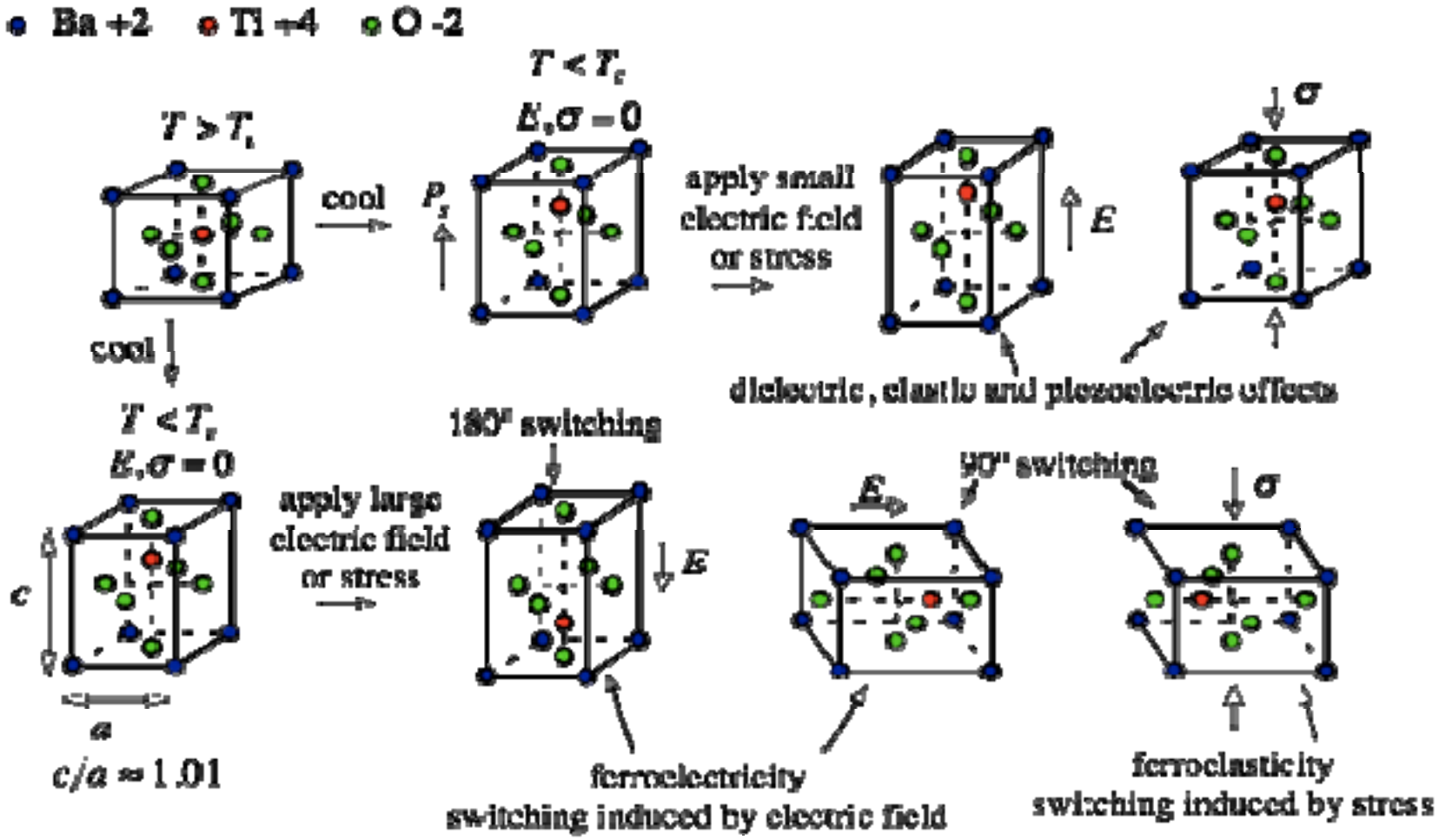


Variants in cubic-tetragonal transition



Variants coexisting as domains

Electromechanical Switching in $BaTiO_3$



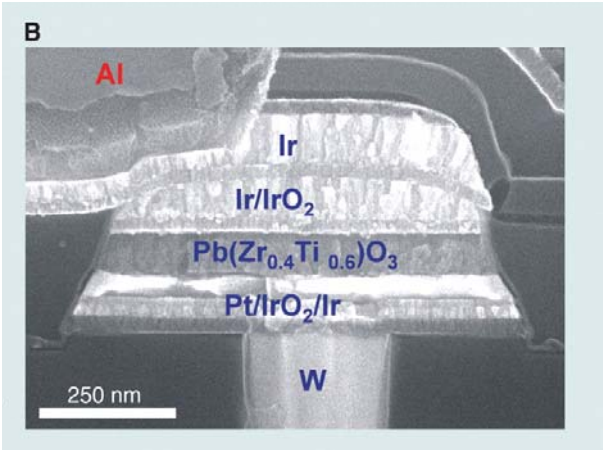
http://www.ae.utexas.edu/~landis/Landis/Research.html

Applications of ferroelectric materials

Bosch Fuel Injector
(piezoelectric)

Ramtron 4MByte FRAM
(Ferroelectric)

Nikitar Zoom Lens
(piezoelectric)



32 Mb Samsung PZT FRAM

Phase field model

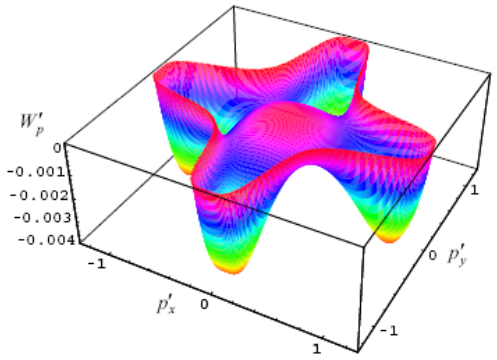
The total potential energy, E, of a Ferroelectric material may be written as

$$E = \int_{\Omega} [U(\nabla \mathbf{p}) + W(\boldsymbol{\varepsilon}, \mathbf{p})] \, \mathrm{d}\Omega + \frac{\varepsilon_0}{2} \int_{R^3} |\nabla \phi|^2 \, \mathrm{d}\Omega.$$

Domain wall energy

$$U(p_{i,j}) = \frac{a_0}{2}(p_{1,1}^2 + p_{1,2}^2 + p_{2,1}^2 + p_{2,2}^2),$$

Ferroelectric Multiwell energy



$$\begin{aligned} W(p_i, \varepsilon_{jk}) = {} & \frac{a_1}{2}(p_1^2 + p_2^2) + \frac{a_2}{4}(p_1^4 + p_2^4) + \frac{a_3}{2}p_1^2 p_2^2 \\ & + \frac{a_4}{6}(p_1^6 + p_2^6) + \frac{a_5}{4}p_1^4 p_2^4 - \frac{b_1}{2}(\varepsilon_{11}p_1^2 + \varepsilon_{22}p_2^2) \\ & - \frac{b_2}{2}(\varepsilon_{11}p_2^2 + \varepsilon_{22}p_1^2) - b_3(\varepsilon_{12} + \varepsilon_{21})p_1 p_2 \\ & + \frac{c_1}{2}(\varepsilon_{11}^2 + \varepsilon_{22}^2) + c_2\varepsilon_{11}\varepsilon_{22} + \frac{c_3}{2}(\varepsilon_{12}^2 + \varepsilon_{21}^2). \end{aligned}$$

where electric potential ϕ is obtained by solving the Maxwell's equation

$$\nabla . (\mathbf{p} - \epsilon_o \nabla \phi) \; = \; \rho$$

Phase Field model continued ….

Gradient flow of E leads to governing equations:

$$\mu \dot{p}_i = \left(\frac{\partial U}{\partial p_{i,j}} \right)_{,j} - \frac{\partial W}{\partial p_i} - \phi_{,i},$$

$$p_{i,i} - \varepsilon_0 \phi_{,ii} = 0,$$

$$\left(\frac{\partial W}{\partial \varepsilon_{ij}} \right)_{,j} = 0$$

As an initial approximation neglect elasticity

Solve for equilibrium values of **p** and ϕ

Reference:
A computational model of ferroelectric domains. Part I: model formulation and domain switching
W. Zhang, K. Bhattacharya, Acta Materialia , Volume 53, Issue 1, 3 January 2005, Pages 185–198

Discretization

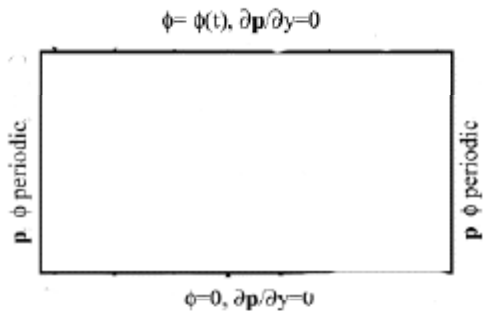
Finite Difference, Explicit Scheme in time, 3 variables per grid point

$$\frac{p_x^{k+1}(i,j)-p_x^k(i,j)}{\Delta t} = \frac{p_x^k(i+1,j)+p_x^k(i-1,j)+p_x^k(i,j+1)+p_x^k(i,j-1)-4p_x^k(i,j)}{h^2} - \frac{\partial W}{\partial p_x}\Big|_{\mathbf{p}^k} - \frac{\phi^k(i+1,j)-\phi^k(i-1,j)}{2h} \tag{2a}$$

$$\frac{p_y^{k+1}(i,j)-p_y^k(i,j)}{\Delta t} = \frac{p_y^k(i+1,j)+p_y^k(i-1,j)+p_y^k(i,j+1)+p_y^k(i,j-1)-4p_y^k(i,j)}{h^2} - \frac{\partial W}{\partial p_y}\Big|_{\mathbf{p}^k} - \frac{\phi^k(i,j+1)-\phi^k(i,j-1)}{2h} \tag{2b}$$

The electric potential is solved for using the Jacobi iteration. The loop update is given by :

$$\phi^{n+1}(i,j) = 0.25\Big\{\phi^n(i+1,j)+\phi^n(i-1,j)+\phi^n(i,j+1)+\phi^n(i,j-1) - \frac{h^2}{\epsilon}\Big(\frac{p_x^n(i+1,j)-p_x^n(i-1,j)}{2h} + \frac{p_y^n(i,j+1)-p_y^n(i,j-1)}{2h}\Big)\Big\}$$



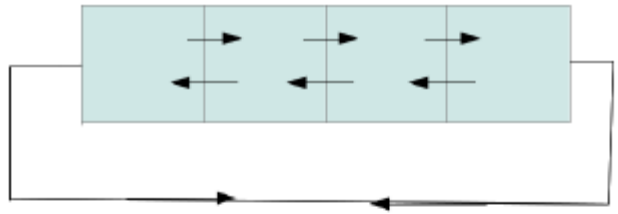
Random initial polarization.

Geometry and boundary conditions used for the simulation

Periodic boundary conditions in lateral direction

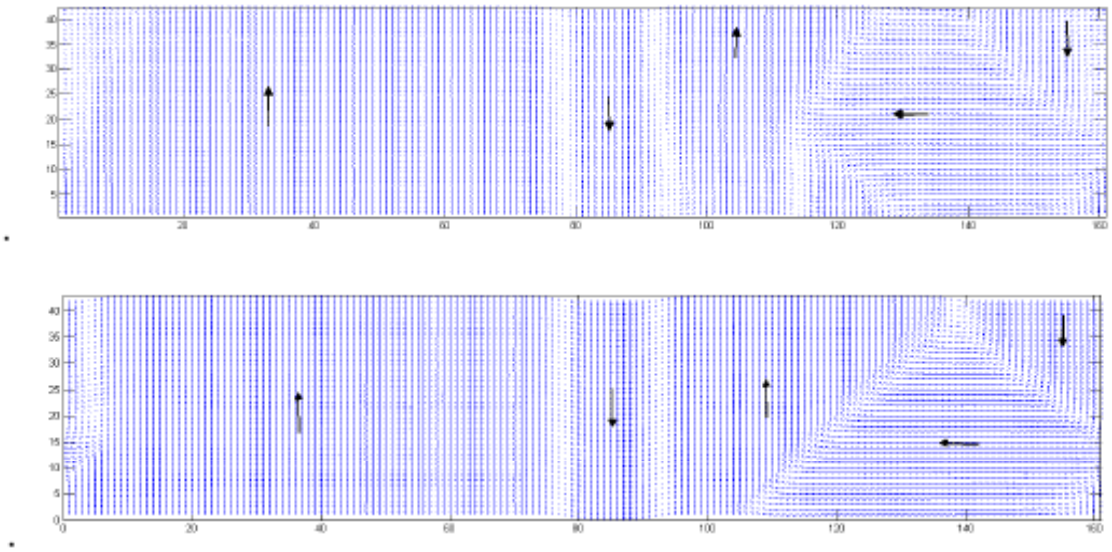
Parallel Implementation

- Finest grain tasks
  Update **p**(i,j) (time update)
  Update ϕ(i,j) (Jacobi update)
- Coarsening (bundle multiple grid points and assign to each process)
- MPI Implementation
- Communication between adjacent processors, Convergence criterion (for both ϕ (each time step, Jacobi) , **p** (at equilibrium)
- Execution built around Homework problem.
- 160 ** 40 grid (resolution depends on domain wall thickness)
- Variables: 3*6400



Layout and Communicaton for 4 processors

Results



Computed domains

Future Work

- Introduce elasticity
- Semiconducting effect (non-linear problem)
- Change geometry (notches)