

PFM and related domain writing

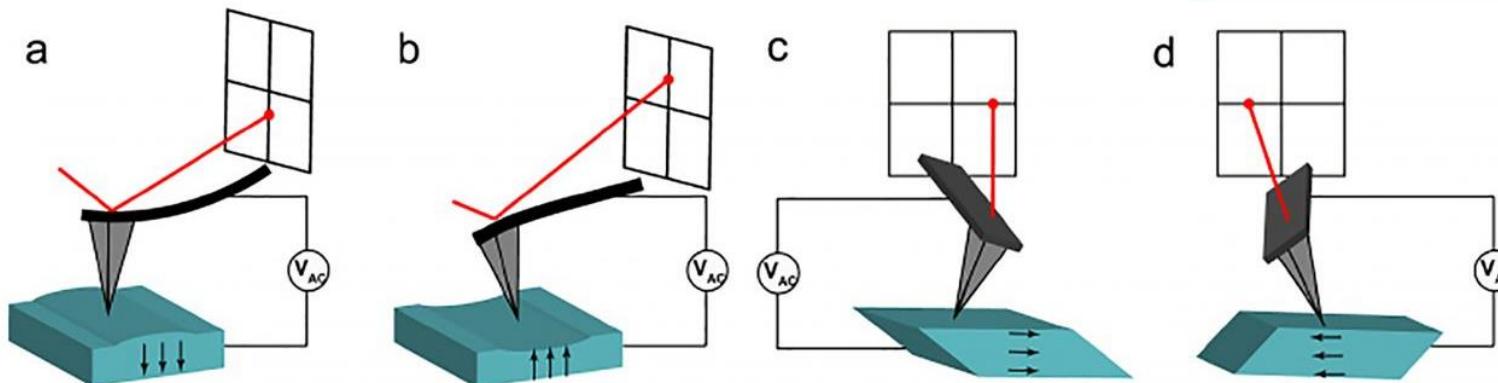
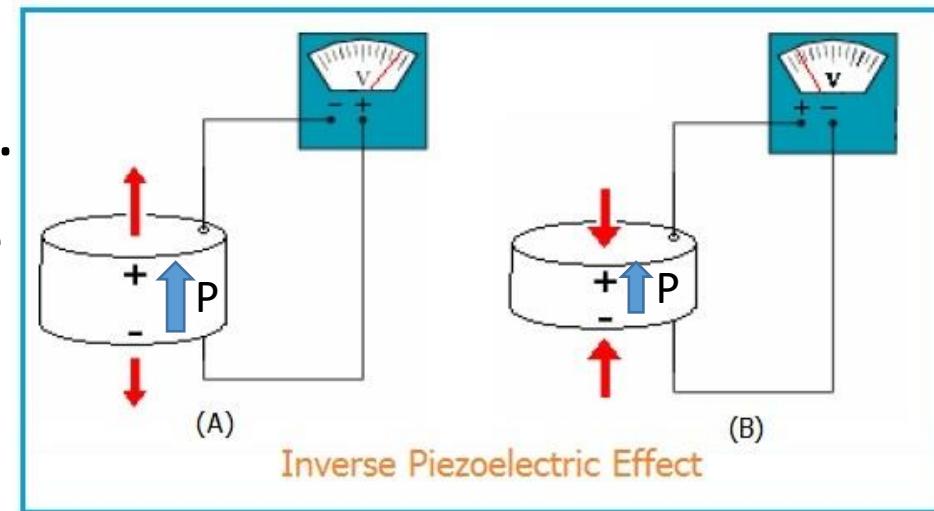
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2019-06-14

Anna N. Morozovska, Eugene A.
Eliseev, Phyica B, 373, 54-63,(2006)

What is PFM?

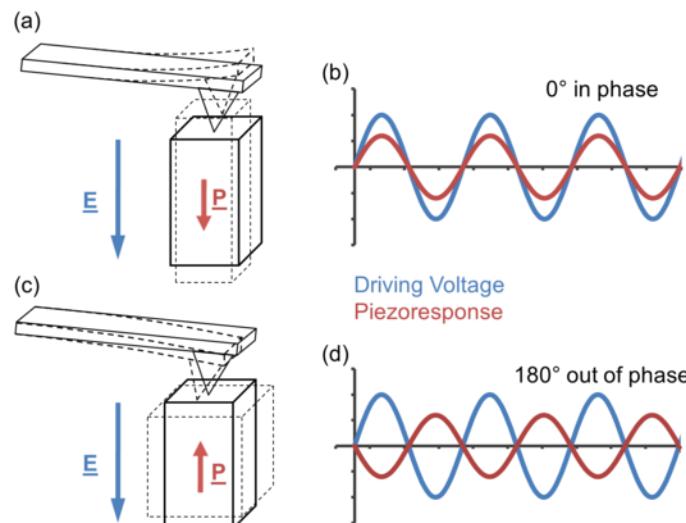
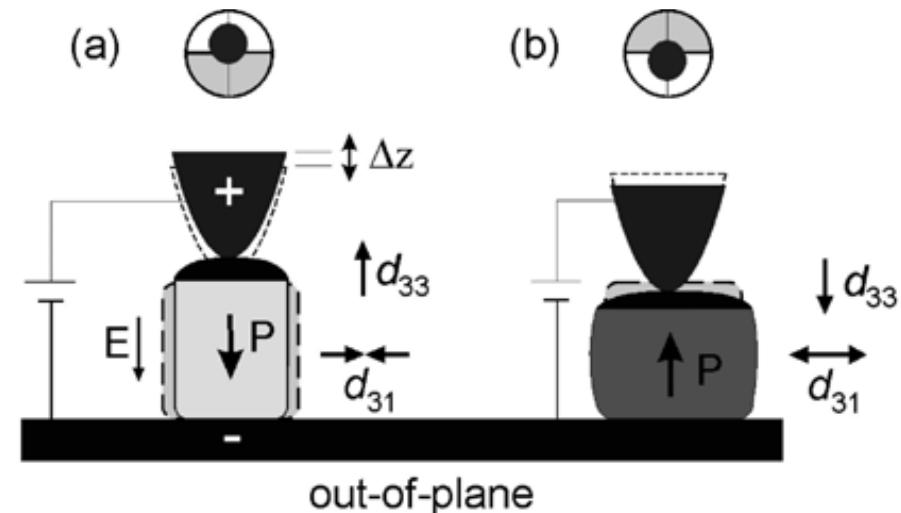
- Piezoresponse force microscopy (PFM) is a local method to detect the sample deformation due to electric field.
- Piezoelectricity: accumulation of charges under mechanical stress.
- Ferroelectric materials usually have Piezoelectric effects.
- Detection of deformation using V_{AC}



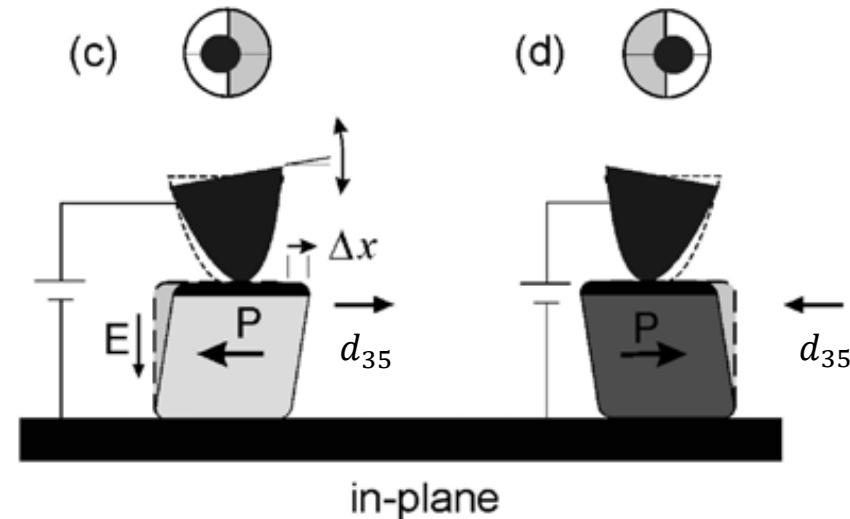
PFM signal from converse piezoelectric effect

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \begin{pmatrix} d_{11} & d_{21} & d_{31} \\ d_{12} & d_{22} & d_{32} \\ d_{13} & d_{23} & d_{33} \\ d_{14} & d_{24} & d_{34} \\ d_{15} & d_{25} & d_{35} \\ d_{16} & d_{26} & d_{36} \end{pmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix}$$

$$d_{ki}^0 = \begin{pmatrix} 0 & 0 & d_{31}^0 \\ 0 & 0 & d_{32}^0 \\ 0 & 0 & d_{33}^0 \\ 0 & d_{24}^0 & 0 \\ d_{15}^0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



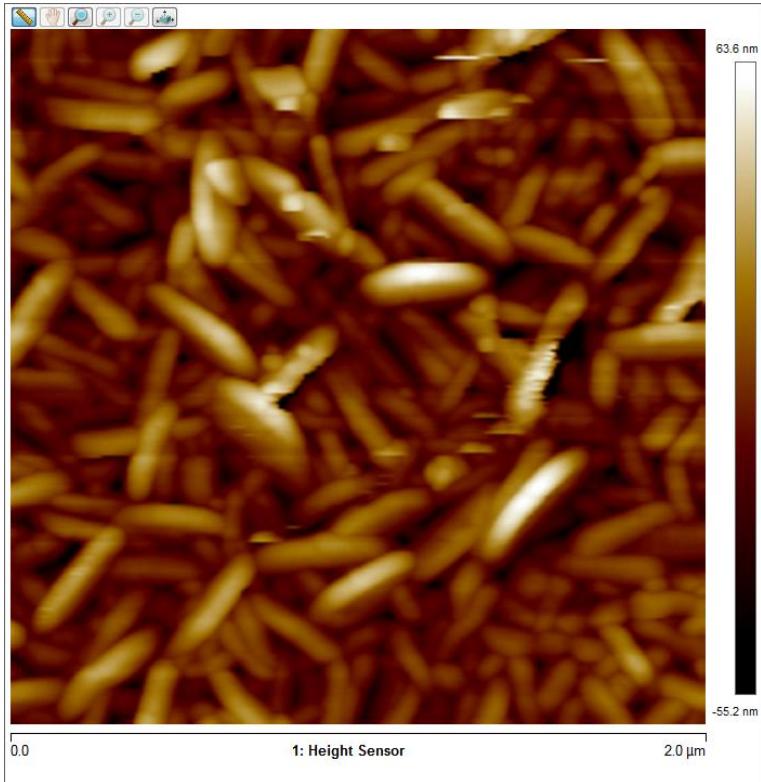
$$d_{ki} = \begin{pmatrix} d_{11} & 0 & 0 \\ d_{12} & 0 & 0 \\ d_{13} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & d_{35} \\ 0 & d_{26} & 0 \end{pmatrix}$$



PFM signal from other sources

Capacitive force

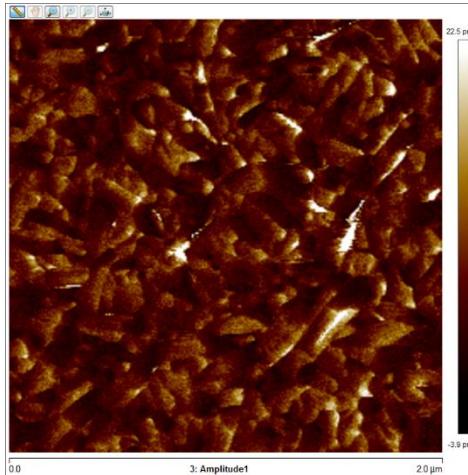
$$F_{cap} = \frac{dW_{cap}}{dz} = \frac{1}{2}V^2 \frac{dC}{dz}$$



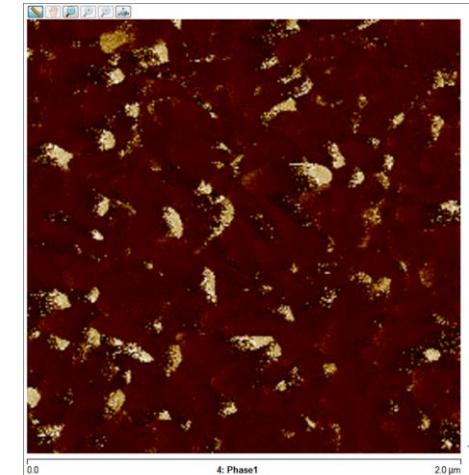
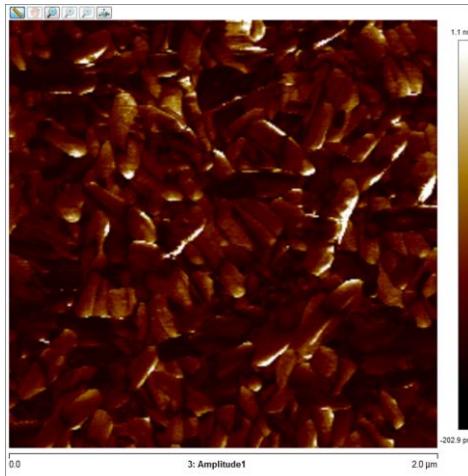
Coulomb force

$$F_{coul} = \frac{\sigma CV}{2\epsilon_0},$$

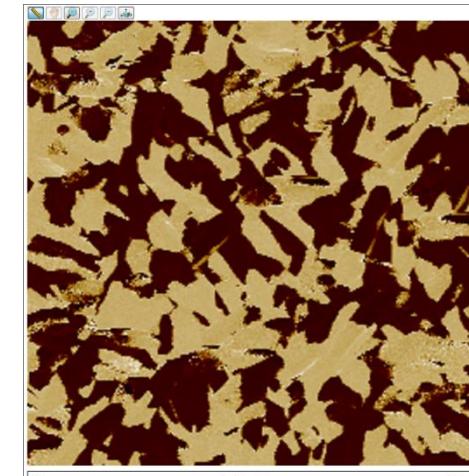
Vertical



Lateral

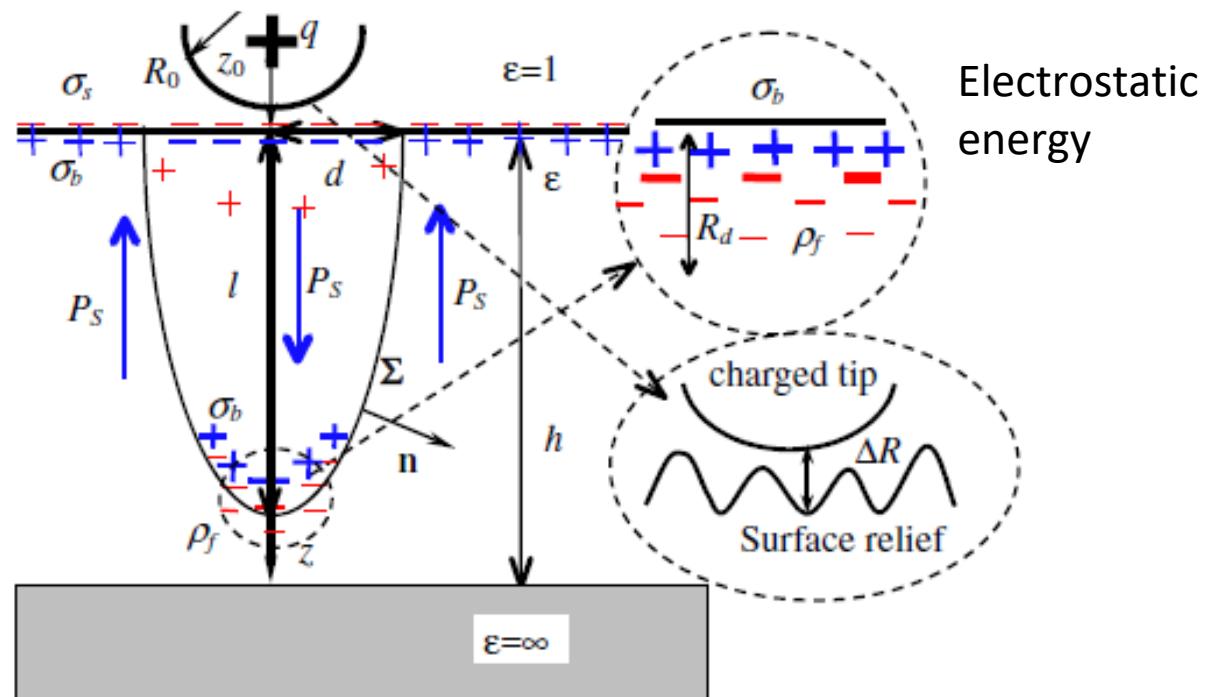


From
morphology



From
FE domains

Domain writing using PFM tip



$$\Phi(d, l) = \Phi_q(d, l) + \Phi_D(d, l) + \Phi_C(d, l).$$

$\Phi_q(d, l)$ is electrostaic energy from point change on tip

$\Phi_D(d, l)$ is depolarization energy from the interface

$\Phi_c(d, l)$ is surface energy at the domain wall

Fig. 2. Domain formation induced by positively charged tip with effective charge q and distance z_0 from the surface, R_0 is tip radius of curvature, ΔR is the distance between the tip apex and the sample surface, d is semiellipsoid radius, l is semiellipsoid major axis, R_d is the thickness of the screening space-charge layer, P_S is spontaneous polarization, σ_s is surface charges captured on the trap levels, σ_b is bound charges related to P_S discontinuity, ρ_f is free charge density. We choose constant spontaneous polarization $+P_S$ inside and $-P_S$ outside the domain. The system as a whole is electro neutral.

φ_q

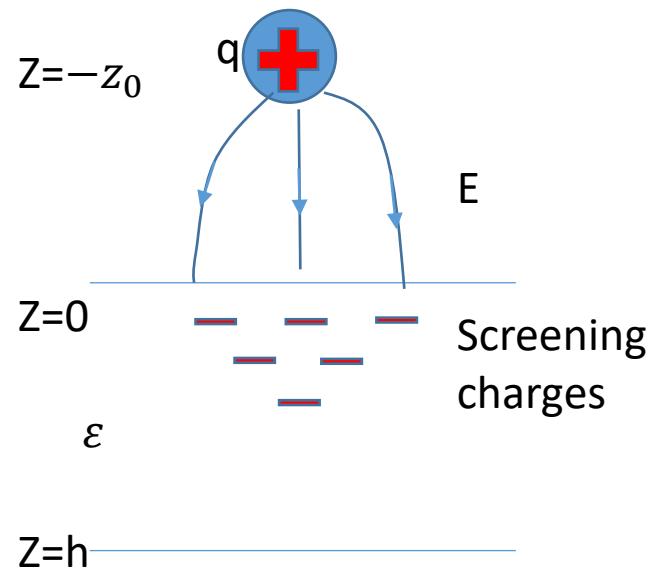
$$\Delta\varphi_0(\mathbf{r}) = -4\pi q\delta(x, y, z + z_0), \quad z \leq 0,$$

$$\Delta\varphi_q(\mathbf{r}) - \frac{\varphi_q(\mathbf{r})}{R_d^2} = 0, \quad 0 \leq z \leq h, \quad \rho_f(\mathbf{r}) \approx -\frac{\varepsilon\varphi(\mathbf{r})}{4\pi R_d^2}, \quad R_d^2 = \frac{\varepsilon k_B T}{4\pi e^2 (Z^2 n_d + n_0)}$$

$$\varphi_0(z = 0) = \varphi_q(z = 0),$$

$$\left(\frac{\partial\varphi_0}{\partial z} - \varepsilon \frac{\partial\varphi_q}{\partial z} \right) \Big|_{z=0} = 0,$$

$$\varphi_q(z = h) = 0.$$



When $\varepsilon \gg 1, \exp(-h/R_d) \ll 1$

$$\begin{aligned} \varphi_q(\mathbf{r}) &\approx 2q \int_0^\infty dk \frac{k \cdot J_0(k\sqrt{x^2 + y^2})}{k + \varepsilon\sqrt{k^2 + R_d^{-2}}} \\ &\quad \times \exp(-z\sqrt{k^2 + R_d^{-2}} - kz_0) \\ &\leq \frac{2q}{\varepsilon + 1} \frac{\exp(-z/R_d)}{\sqrt{x^2 + y^2 + (z_0 + z)^2}}. \end{aligned}$$

φ_D

$$\Delta\varphi_{\text{DE}}(\mathbf{r}) - \frac{\varphi_{\text{DE}}(\mathbf{r})}{R_d^2} = 0,$$

$$\varepsilon \left(\frac{\partial \varphi_{\text{DE int}}}{\partial n} - \frac{\partial \varphi_{\text{DE ext}}}{\partial n} \right) \Big|_{\Sigma} = 8\pi (\mathbf{P}_S \mathbf{n})|_{\Sigma},$$

$$\varphi_{\text{DE}}(z=0) = 0.$$

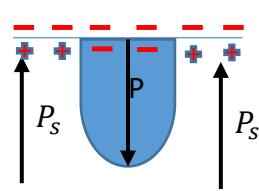
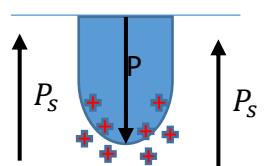
$$\Delta\varphi_{D0}(\mathbf{r}) = 0, \quad z \leq 0,$$

$$\varphi_{D0}(z=0) = \varphi_{\text{DS}}(z=0),$$

$$\left(\frac{\partial \varphi_{D0}}{\partial z} - \varepsilon \frac{\partial (\varphi_{\text{DS}} + \varphi_{\text{DE}})}{\partial z} \right) \Big|_{z=0}$$

$$= \begin{cases} -8\pi P_S, & \sqrt{x^2 + y^2} < d, \\ 0, & \sqrt{x^2 + y^2} > d, \end{cases}$$

$$\Delta\varphi_{\text{DS}}(\mathbf{r}) - \frac{\varphi_{\text{DS}}(\mathbf{r})}{R_d^2} = 0, \quad 0 \leq z.$$



$$\varphi_{\text{DE}}(\mathbf{r}) \leq \begin{cases} \frac{8\pi P_S}{\varepsilon} \frac{d^2}{l^2} \left(\operatorname{arcth} \left(\sqrt{1 - \frac{d^2}{l^2}} \right) - 1 \right) \\ \times \exp \left(-\frac{l - \sqrt{z^2 + l^2(x^2 + y^2)/d^2}}{R_d} \right) z, & s \leq 0, \\ \frac{8\pi P_S}{\varepsilon} \frac{d^2}{l^2} \left(\operatorname{arcth} \left(\sqrt{\frac{l^2 - d^2}{s + l^2}} \right) - \frac{l}{\sqrt{s + l^2}} \right) \\ \times \exp \left(-\frac{\sqrt{z^2 + l^2(x^2 + y^2)/d^2} - l}{R_d} \right) z, & s \geq 0. \end{cases} \quad (\text{B.5})$$

Here $s(x, y, z)$ is the one of ellipsoidal coordinates $(x^2 + y^2)/(d^2 + s) + z^2/(l^2 + s) = 1$ ($s = 0$ corresponds to the boundary of domain).

$$\begin{aligned} \varphi_{\text{DS}}(\mathbf{r}) \sim & -4\pi P_S d^2 \int_0^\infty dk \frac{k J_0(k \sqrt{x^2 + y^2})}{k + \varepsilon \sqrt{k^2 + R_d^{-2}}} \\ & \times \exp(-z \cdot \sqrt{k^2 + R_d^{-2}}). \end{aligned}$$

$$\Phi_q, \Phi_D, \Phi_C$$

$$\Phi_q(d, l)$$

$$= \int_{\Sigma(z>0)} ds(\mathbf{P}_S \cdot \mathbf{n}) \varphi_q - \int_{\substack{(x^2+y^2) \leq d^2 \\ z=0}} dx dy \varphi_q P_S \\ - \frac{\varepsilon}{4\pi R_d^2} \int_{z>0} dv \varphi_D \varphi_q + \frac{q}{2} \varphi_{D0}(r_0)$$

$$\approx \begin{cases} \frac{8\pi}{\varepsilon} P_S q R_d \frac{(z_0 - \sqrt{z_0^2 + d^2})}{2\sqrt{z_0^2 + d^2}} \\ + O\left(\left(\frac{d}{l}\right)^2 \exp(-l/R_d)\right), \quad R_d \rightarrow 0, \\ \frac{8\pi}{\varepsilon} P_S q (z_0 - \sqrt{z_0^2 + d^2}) \\ + O\left(\left(\frac{d}{l}\right)^2 \exp(-l/R_d)\right), \quad R_d \rightarrow \infty. \end{cases}$$

$$\Phi_C(d, l) = \pi d^2 \psi_S + \pi dl \psi_S \frac{1}{\sqrt{1 - (d/l)^2}} \\ \times \arcsin\left(\sqrt{1 - (d/l)^2}\right) \approx \frac{\pi^2}{2} \psi_S dl.$$

$$\Phi_{DV}(d, l)$$

$$= \int_{\Sigma(z>0)} ds(\mathbf{P}_S \cdot \mathbf{n}) \varphi_{DE} - \frac{\varepsilon}{8\pi R_d^2} \int_{z>0} dv \varphi_{DE}^2 \\ = \begin{cases} \frac{16\pi^2 P_S^2}{3\varepsilon} \frac{d^4}{l} (\ln(2l/d) - 1), & R_d \rightarrow \infty, \\ \frac{4\pi^2 P_S^2}{\varepsilon} d^2 R_d, & R_d \rightarrow 0. \end{cases}$$

$$\Phi_{DS}(d, l)$$

$$= \int_{\Sigma(z>0)} ds(\mathbf{P}_S \cdot \mathbf{n}) \varphi_{DS} - \int_{\substack{(x^2+y^2) \leq d^2 \\ z=0}} dx dy \varphi_{DS} P_S \\ - \frac{\varepsilon}{8\pi R_d^2} \int_{z>0} dv (\varphi_{DS}^2 + 2\varphi_{DS}\varphi_{DE}) \\ = \int_{V_\Sigma} dv P_S \frac{d\varphi_{DS}}{dz} - \frac{\varepsilon}{8\pi R_d^2} \int_{z>0} dv (\varphi_{DS}^2 + 2\varphi_{DS}\varphi_{DE}).$$

ψ_S is surface energy

Domain dimension vs V_{DC}

$$\Phi(d, l) = \Phi_q(d, l) + \Phi_D(d, l) + \Phi_C(d, l).$$

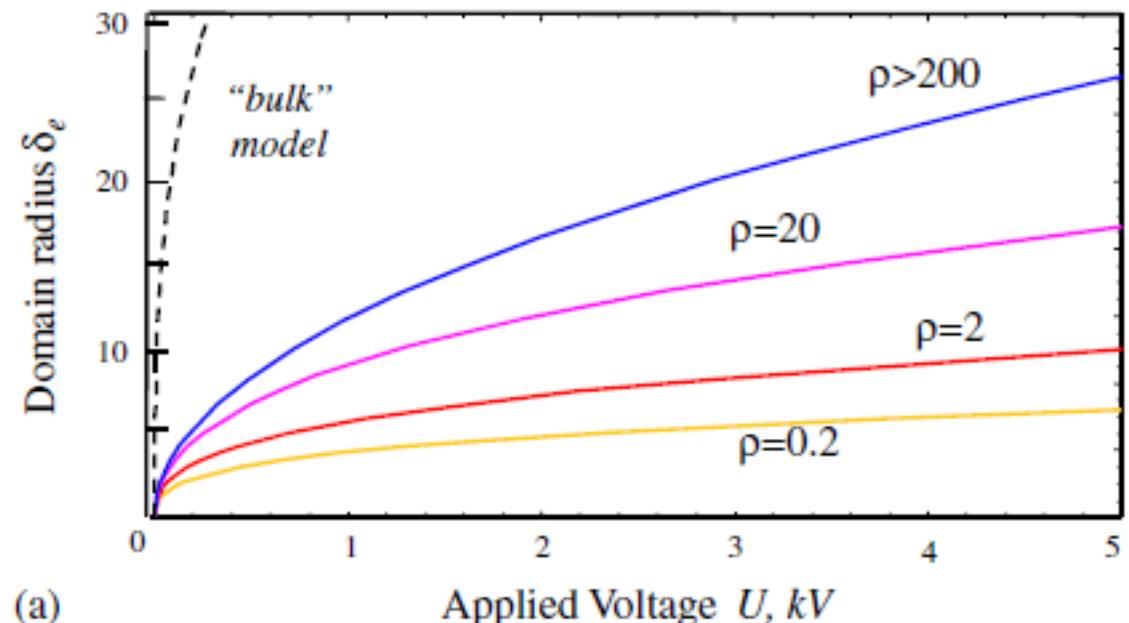
$$\delta = \frac{d}{R_0}, \lambda = \frac{l}{R_0}, \rho = \frac{R_d}{R_0}$$

$$\begin{cases} \frac{\partial \Phi(\delta, \lambda)}{\partial \lambda} = 0, & \frac{\partial \Phi(\delta, \lambda)}{\partial \delta} = 0, \\ \frac{\partial^2 \Phi(\delta, \lambda)}{\partial^2 \lambda} > 0, & \frac{\partial^2 \Phi(\delta, \lambda)}{\partial^2 \delta} > 0. \end{cases}$$

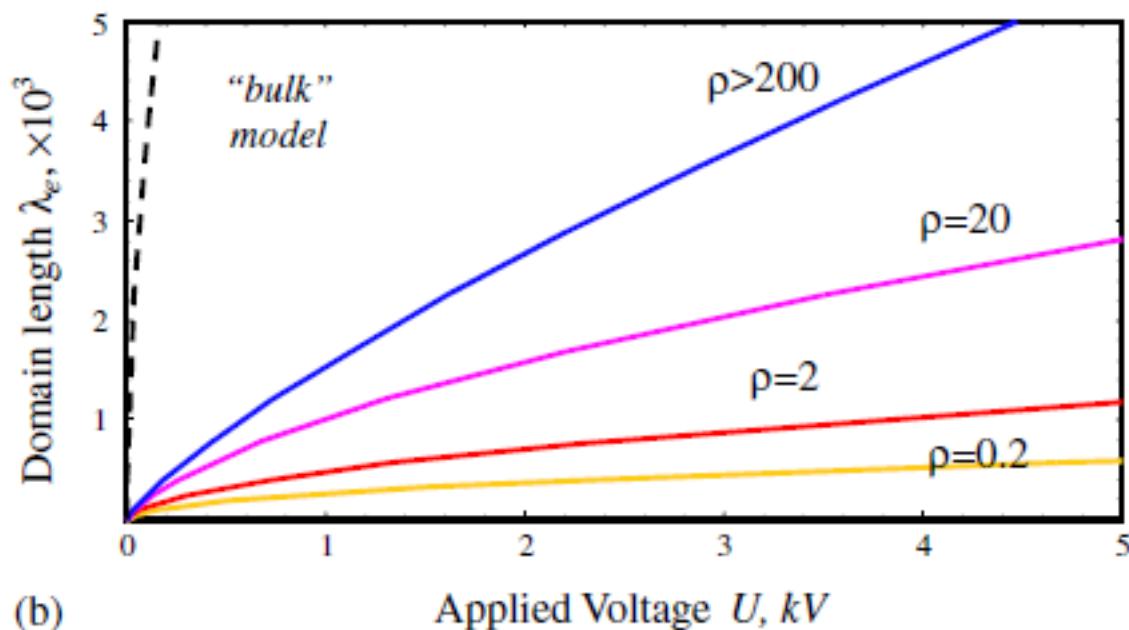
For the usual case $3\lambda_e\rho \gg 4\delta_e^2$ and $W_C \ll W_D$ we found the following approximate equations:

$$\begin{aligned} \lambda_e &= \delta_e^{3/2} \sqrt{\frac{W_D}{W_C} (\ln(2\lambda_e/\delta_e) - 2)} \\ &\approx \delta_e^{3/2} \sqrt{\frac{W_D}{W_C} \left(\ln \left(2\sqrt{\frac{W_D}{W_C}} \delta_e \right) - 2 \right)}, \end{aligned} \quad (13a)$$

$$\begin{aligned} W_q &\approx \left(W_D \left(\frac{3\pi\delta_e\rho/4 + 8\delta_e^2/3}{(\pi\rho/4 + 4\delta_e/3)^2} - \frac{\delta_e^2}{\lambda_e\rho} \right) + W_C \frac{\lambda_e}{\delta_e\rho} \right) \\ &\times \frac{\sqrt{\delta_e^2 + \xi^2}}{(\rho + 2\xi)} (\rho + 2\sqrt{\delta_e^2 + \xi^2})^2. \end{aligned} \quad (13b)$$



(a)



(b)