ECE215B/Materials206B Winter 2008
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Homework #1 Solutions

1) **Silicon capacitor**: The potential energy can be expressed as

$$U=\frac{V}{2}\varepsilon_0 E_0^{\,2}+\int_0^{E_{in}} \vec{E}'_{in}\, d\left(\vec{P}'\cdot V\right)$$

where V is the sample volume, E_0 is the magnitude of the field that would exist in the absence of the solid, and E' and P' are the dummy electric-field and polarization vector variables. Since the solid is inside a metallic parallel-plate capacitor (i.e., a Si sample with metal plates on the surface), $\vec{E}_0=\vec{E}_{in}$. Furthermore, we can assume that $\vec{E}_{in}$ and $\vec{P}_{in}$ are both uniform so that $d\left(\vec{P}_e\cdot V\right)=V\cdot d\vec{P}_e$. And if we consider Si as a good dielectric, $\vec{P}_e \approx \varepsilon_0\chi_e\vec{E}_{in}$ so that

$$U'=\frac{U}{V}=\frac{1}{2}\varepsilon_0 E_{in}^{\,2}+\varepsilon_0\chi_e\int_0^{E_{in}}\vec{E}'_{in}\cdot d\vec{E}'_{in}=\frac{1}{2}\varepsilon_0 E_{in}^{\,2}\left(1+\chi_e\right)=\frac{1}{2}\varepsilon_0\varepsilon_r E_{in}^{\,2}$$

a) The maximum U' occurs when $\boldsymbol{E}_{in}=\boldsymbol{E}_{\max}$, so that

$$\left[U'\right]^{\max}=4.8\times10^{4}\ J/m^3=4.8\times10^{-2}\ J/cm^3 \quad \text{for } \varepsilon=12,\ E_{max}=3\text{x}10^7\ \text{V/cm}$$

b) The maximum polarization per unit volume is simply

$$P_e^{\max}=\varepsilon_0\chi_e E_{max}=2.9\times10^{-3}\ \text{Cb}/\text{m}^2 \quad \text{for } \chi_e=\varepsilon_r-1=11$$

2. (**Atomic polarizability**). Diamond, silicon, and germanium

(a)	Si	Ge	C (diamond)
ε_r	11.7	15.8	5.5
Atomic concentration [m^{-3}]	5.00E+28	4.42E+28	1.76E+29

(b)	Si	Ge	C (diamond)
$(\varepsilon_r-1)/(\varepsilon_r+2)$	7.81E-01	8.31E-01	6.00E-01
Polarizability, [Cb-m^2/V]	4.147E-40	4.994E-40	9.051E-41

(c)	Si	Ge	C (diamond)
atomic radius [A]			
$R=(\alpha/4\pi\varepsilon_0)^{1/3}$	1.55	1.65	0.93

(d)	Si	Ge	C (diamond)
Nearest neighbor distance [Ang], R_{nn}	2.35	2.45	1.54
Half nearest neighbor distance, $R_{nn}/2$	1.18	1.23	0.77
$R_{nn}/(2R_0)$	0.76	0.74	0.82

3. (Ionic polarizability): KI and MgO

(a)	KI	MgO
Nearest neighbor separation [Ang]	3.533	2.1
Unit cell constant [Ang]	7.066	4.2
Unit cell volume [m^3]	3.52794E-28	7.4088E-29
Stiffness coeff C11 [N/m^2]	2.740E+10	2.860E+11

(b)	KI	MgO
Density [KG/m^3]	3142.95	3634.02
Speed of sound [m/s]	2952.61	8871.34
q/e	1	2
α	2.65E-39	1.71E-39

Note in (b) that MgO is bivalent, i.e., each ion is doubly charged

(c)	KI	MgO
χ_e ($\approx n^*\alpha/\varepsilon_0$)	3.40	10.4
Calculated εr	4.40	11.4
*Accepted εr	5.10	9.65

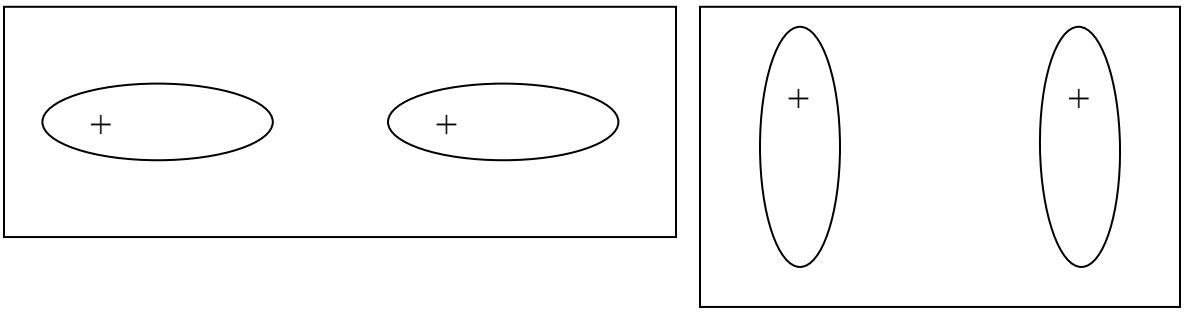
www.crystran.co.uk/kidata.htm*

4. Ferroelectric criterion for atoms, two neutral atoms of polarizability α, and separation a.

Ferroelectric criterion is the "self-consistent " criterion for spontaneous polarization: that the electric field at a given atom caused by all the neighboring polarized atoms (moment $\vec{p}$) is equal to the electric field required to polarize the given atom to moment $\vec{p}$ (sounds like "double talk", but that's what self-consistency is all about). This allows for a spontaneous polarization in the absence of external fields.

Consider two alignments of atomic dipoles:

1) atomic dipoles collinear: parallel but not collinear:

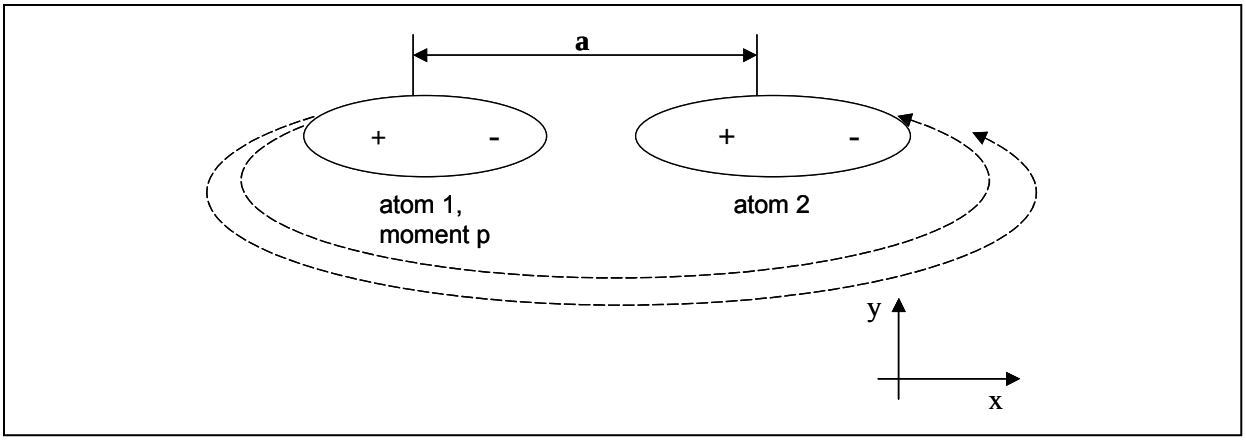


Independent of orientation, $\vec{E}$ from dipole is: $\dfrac{3(\vec{p}\cdot\vec{r})\vec{r} - r^2\vec{p}}{4\pi\varepsilon_0 r^5}$.

a) for co-linear dipoles:

Field on atom 2 from atom 1 is $\vec{E}_{21} = \dfrac{2p_1}{4\pi\varepsilon_0 a^3}(-\hat{x})$. Induced dipole moment on atom 2 is $\vec{p}_2 = \alpha\vec{E}_{21} = \dfrac{2\alpha p_1}{4\pi\varepsilon_0 a^3}(-\hat{x})$. But the fact that $\vec{p}_1$ *and* $\vec{p}_2$ are co-linear

$\Rightarrow |\vec{p}_2| = p = \dfrac{2\alpha p_1}{a^3} = \dfrac{2\alpha p}{4\pi\varepsilon_0 a^3}$ *or* $\alpha = 2\pi\varepsilon_0 a^3$



b) for atomic dipoles parallel but not collinear: in this case, the filed at atom 2 caused by dipole at atom 1 is always pointed opposite to dipole direction at atom 1.

So atomic dipoles cannot co-align on the fields from neighboring dipoles $\Rightarrow$ no ferroelectricity for just two atoms along this direction.