ELEG 667–016; MSEG-667-016 - Solid State Nanoelectronics – Fall 2005
Solution
Homework #3 - due Thursday, 22 September 2005, in class

1. **Ferroelectric criterion for atoms:** Consider a system of two neutral atoms separated by a fixed distance $\boldsymbol{a}$, each atom having a polarizability $\boldsymbol{\alpha}$. Find the relation between $\boldsymbol{a}$ and $\boldsymbol{\alpha}$ for such a system to be ferroelectric. *Hint:* The dipolar field is strongest along the axis of the dipole.

2. **Saturation polarization at Curie point:** In a first-order transition, the equilibrium condition:
$(T-\Theta)/C - |g_4|P_s^2 + g_6P_s^4 = 0$
with T set equal T_c gives one equation for the polarization $P_s(T_c)$ at the transition temperature. A further condition at the Curie point is that $F(P_s,T_c) = F(0,T_c)$.
(a) Combining these two conditions, show that $P_s^2(Tc) = 3|g_4| / 4g_6$.
(b) Using this result, show that $T_c = \Theta + 3\ C\ g_4^2 / 16g_6$.

Solutions:
1. For field along z axis due to $\boldsymbol{p}_1$; $E_z(\text{at } \boldsymbol{p}_2) = 2\boldsymbol{p}_1/a^3$. $\boldsymbol{p}_2 = \alpha E_z = 2\alpha\boldsymbol{p}_1/a^3$. This has solution $p_1 = p_2 \neq 0$ if $2\alpha = a^3$; $\alpha = \frac{1}{2}a^3$.

2. (a). One condition is, from the minimization,

$$\gamma\left(T_C - T_0\right) - |g_4|P_s^2 + g_6P_s^4 = 0 .$$

The other condition is

$$\frac{1}{2}\gamma\left(T_c - T_0\right)P_s^2 - \frac{1}{4}|g_4|P_s^4 + \frac{1}{6}g_6P_s^6 = 0 .$$

Thus

$$-|g_4|P_s^2 + g_6P_s^4 = -\frac{1}{2}|g_4|P_s^2 + \frac{1}{3}g_6P_s^4 \ ;$$
$$\frac{2}{3}g_6P_s^2 = \frac{1}{2}|g_4| \ ; \ P_s^2 = \frac{3}{4}\frac{|g_4|}{g_6} .$$

(b) From the first line of part (a),

$$\gamma\left(T_c - T_0\right) = \frac{3}{4}\frac{|g_4|^2}{g_6} - \frac{9}{16}\frac{|g_4|^2}{g_6} = \frac{3}{16}\frac{g_4^2}{g_6} .$$