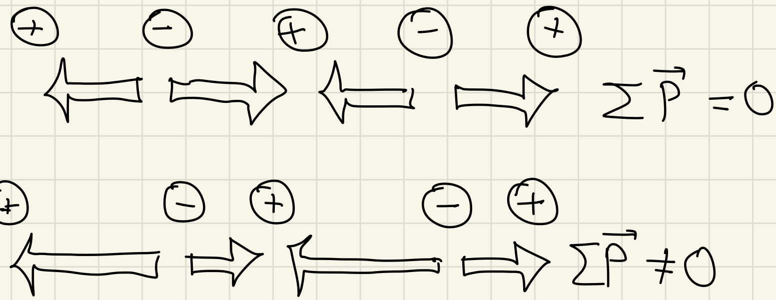
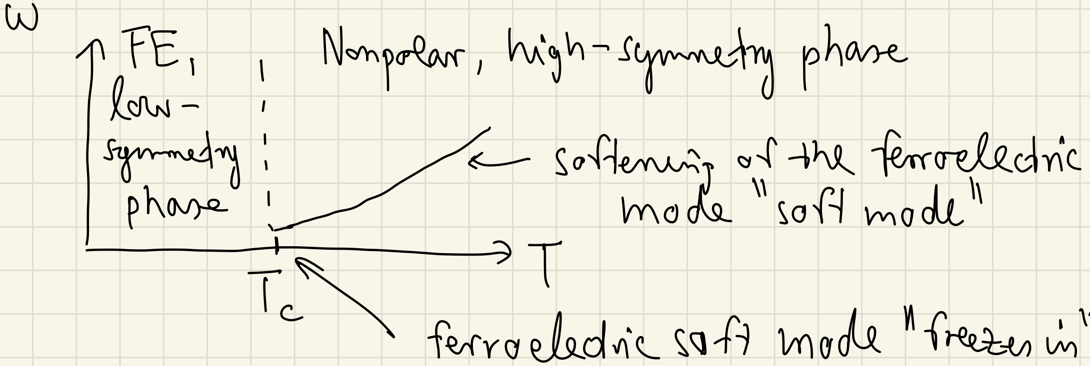
Exercise 3: Primer on ferroelectricity

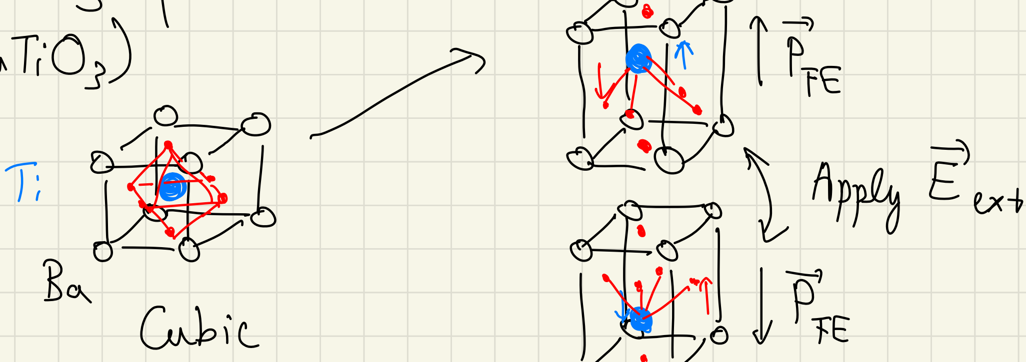
MgO





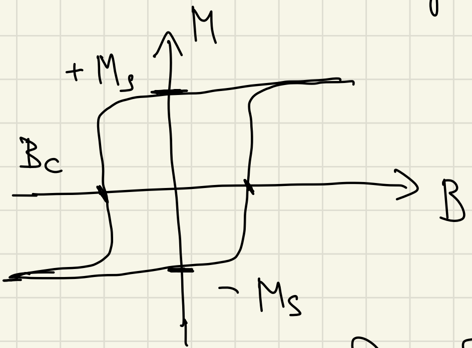
Ferroelectricity arises in ionic solids through inversion-symmetry breaking below a certain transition temperature.

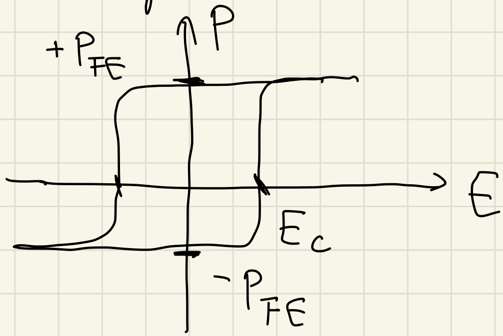
ABO_3 "perovskite" structure
($BaTiO_3$)



Cubic
high-T phase

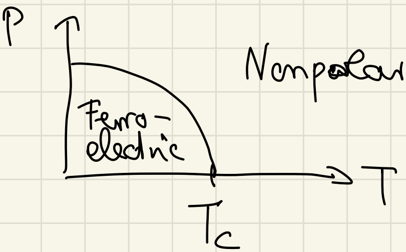
Similiar to ferromagnetism: Hysteresis

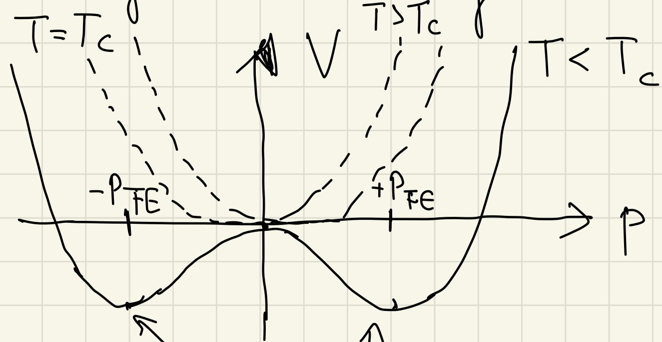




B_c, E_c coercive field strengths

Phase transition: Ginsburg-Landau theory





degenerate minima, between which the material can be switched

Polynamial

$$V(P) = \alpha(T)\, P^2 + \beta(T)\, P^4 = \begin{cases} T>T_c,\ \alpha,\ \beta>0 \\ T<T_c,\ \alpha<0, \beta>0 \end{cases}$$

Calculation of the ferroelectric polarization can be done on the unit-cell level, by comparing the distorted FE structure with its high-symmetry one:

$$\vec{P}_{FE} = \frac{1}{V_c} \sum_n \underline{\underline{Z}}^*_n \vec{u}_n \qquad \vec{u}_n = \vec{u}_{FE,n} - \vec{u}_{high\text{-}symmetry,n}$$