微晶尺寸的计算

假设某一微晶的(hkl)面共有N层，面间距为d，光程差为Δl.

$\Delta l = 2d\sin\theta = \lambda$

$\Delta l = 2d\sin(\theta+\varepsilon) = \lambda + 2\varepsilon d\cos\theta$

相位差：$\Delta\phi = \frac{2\pi\Delta l}{\lambda} = 2\pi + \frac{4\pi\varepsilon d\cos\theta}{\lambda} = \frac{4\pi\varepsilon d\cos\theta}{\lambda}$

N层(hkl)面总的散射振幅为：$E = E_0\sum_{k=0}^{N-1} e^{ik\Delta\phi}$

$I = I_0\frac{\sin^2\frac{N}{2}\Delta\phi}{\sin^2\frac{1}{2}\Delta\phi} = I_0\frac{N^2\sin^2\frac{N}{2}\Delta\phi}{(\frac{N}{2}\Delta\phi)^2}$

当$\varepsilon = 0$时，$I_{max} = I_0 N^2$.　　$\frac{I_{1/2}}{I_{max}} = \frac{1}{2} = \frac{\sin^2\frac{\alpha}{2}}{(\frac{\alpha}{2})^2}$.

当$\varepsilon = \varepsilon_{1/2}$时，$I_{1/2} = \frac{1}{2}I_{max}$

其中$\alpha = 4\pi N\varepsilon_{1/2}d\cos\theta/\lambda$.

从$\frac{\sin^2\frac{\alpha}{2}}{(\frac{\alpha}{2})^2}$对$\frac{\alpha}{2}$作图，当$\frac{\alpha}{2} = 1.40$时，$\varepsilon_{1/2} = \frac{1.40\lambda}{2\pi Nd\cos\theta}$

$\beta_{hkl} = 4\varepsilon_{1/2}$　∴ $\beta_{hkl} = \frac{0.89\lambda}{Nd\cos\theta} = \frac{0.89\lambda}{D_{hkl}\cos\theta}$.

$D_{hkl} = \frac{0.89\lambda}{\beta_{hkl}\cos\theta}$.　—— scherrer公式. 表示垂直(hkl)面的平均尺度.

倒空间的描述：

$\Delta g \propto \frac{k}{d_0}$.　倒空间的倒易矢量的变化量与面间距成反比.

在某应力作用下，该晶粒的衍射线位移与衍射线的级数有关.

微观应力的计算

平均微观应变：$\varepsilon_{平} = (\frac{\Delta d}{d})_{平}$.　$\Delta 2\theta_2 = 2\theta_2 - 2\theta_0 = 2\theta_0 - 2\theta_1$

$\beta = 4\Delta\theta$.　　$\frac{\Delta d}{d} = -\operatorname{ctg}\theta\cdot\Delta\theta$.　∴ $(\frac{\Delta d}{d})_{平} = \frac{\beta}{4}\operatorname{ctg}\theta$.