

Problem Set #3, 12/10/2013,

1. Silver is FCC, $a=4.09\text{\AA}$. A diffractometer tracing of the powder pattern of silver at 27C is made using MoK_α radiation. Let f be the atomic scattering factor, and the LP is the Lorentz-polarization factor. Numbers proportional to the peak areas divided by $f^2(\text{LP})$ are as follows.

hkl	331	422	531	
$A/f^2(\text{LP})$	3.15	2.83	4.45	

- A) From these data determine $2B$ for silver at 27C. The quantity $2B$ is defined by $2M=2B(\sin\theta/\lambda)^2$
- B) From the Debye temperature for silver $\Theta=210\text{C}$, calculate $2B$ for silver at 27C.
- C) By what fraction is the integrated intensity of the (531) reflection reduced by the temperature factor at 27C?
- D) What is the root mean square component of displacement $\langle u_s^2 \rangle^{1/2}$ in silver at 27C?
- E) What is the ratio of $\langle u_s^2 \rangle^{1/2}$ at 27C to the nearest neighbor distance in silver?

2. In the zinc blend type structure, α positions are at 000, $1/2\ 1/2\ 0$, $1/2\ 0\ 1/2$, $0\ 1/2\ 1/2$, and β positions are $1/4\ 1/4\ 1/4$, $3/4\ 3/4\ 1/4$, $3/4\ 1/4\ 3/4$, $1/4\ 3/4\ 3/4$. Assume a nonstoichiometric composition x_a , x_b , and partial long-range order S

- a) In terms of f_a , f_b , x_a , x_b , and S , deduce expressions for F^2 for $h+k+l=\text{odd}$, $h+k+l=2(2n+1)$, $h+k+l=4n$.
- b) If $x_a=0.60$, $x_b=0.40$ what is the maximum possible value of S ? If $x_a=0.60$, $x_b=0.40$, and $S=0.70$, what fraction of the α -positions are correctly occupied?