

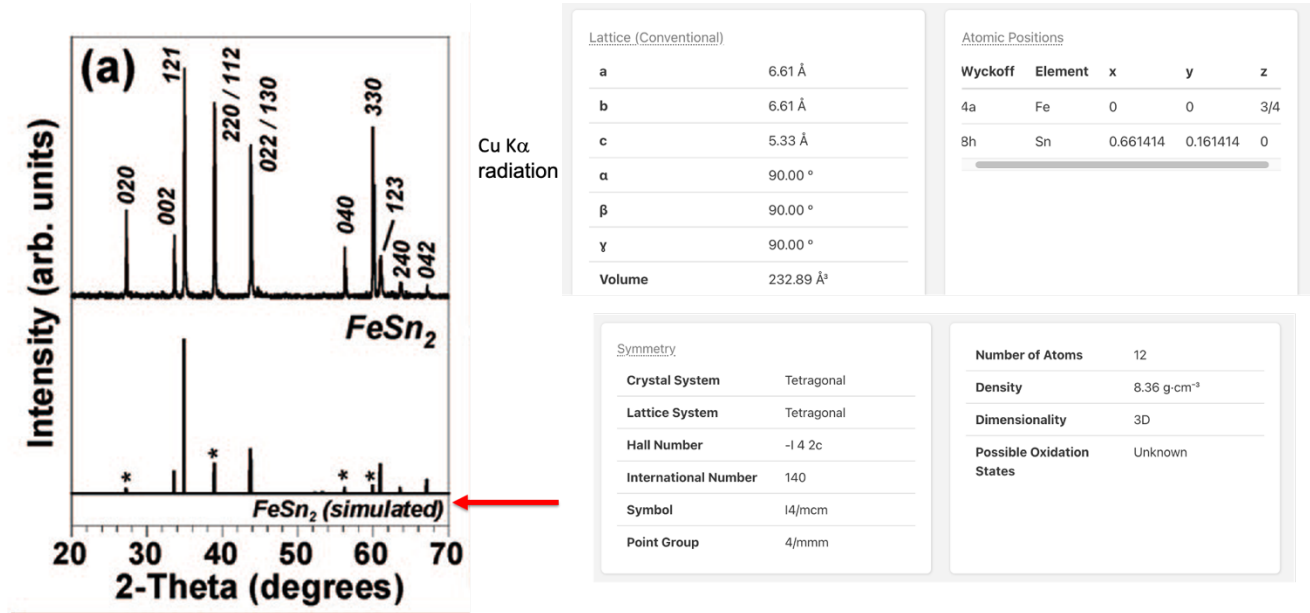
NAME _____

HW 9 See website for due date (include this sheet with your answers)

Prof. S. H. Garofalini

Using the figures below, answer the following questions: (**Typewritten text and equations**)

1. Set up the calculation of the simulated XRD pattern for the (121) and (002) planes by filling in the appropriate equation(s) (no need to actually solve the equation(s)).
2. The simulated pattern below is accurate. What is the implication that the actual pattern (top) differs from the simulated one?



CONTINUED

No. 140

I4/mcm

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$

32	<i>m</i>	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{y}, x, z	(4) y, \bar{x}, z
			(5) $\bar{x}, y, \bar{z} + \frac{1}{2}$	(6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$
			(9) $\bar{x}, \bar{y}, \bar{z}$	(10) x, y, \bar{z}	(11) y, \bar{x}, \bar{z}	(12) \bar{y}, x, \bar{z}
			(13) $x, \bar{y}, z + \frac{1}{2}$	(14) $\bar{x}, y, z + \frac{1}{2}$	(15) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(16) $y, x, z + \frac{1}{2}$

Reflection conditions

General:

$hkl: h + k + l = 2n$
 $hko: h + k = 2n$
 $OkI: k, l = 2n$
 $hhl: l = 2n$
 $00l: l = 2n$
 $h00: h = 2n$

Special: as above, plus

no extra conditions

no extra conditions

$hkl: l = 2n$

$hkl: l = 2n$

no extra conditions

$hkl: l = 2n$

$hkl: l = 2n$

$hkl: k, l = 2n$

$hkl: l = 2n$

$hkl: l = 2n$

$hkl: l = 2n$

$hkl: l = 2n$

16	<i>l</i>	$\dots m$	$x, x + \frac{1}{2}, z$	$\bar{x}, \bar{x} + \frac{1}{2}, z$	$\bar{x} + \frac{1}{2}, x, z$	$x + \frac{1}{2}, \bar{x}, z$
			$\bar{x}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$x + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x}, \bar{z} + \frac{1}{2}$

16	<i>k</i>	$m \dots$	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{y}, x, 0$	$y, \bar{x}, 0$
			$\bar{x}, y, \frac{1}{2}$	$x, \bar{y}, \frac{1}{2}$	$y, x, \frac{1}{2}$	$\bar{y}, \bar{x}, \frac{1}{2}$

16	<i>j</i>	$\dots 2 \dots$	$x, 0, \frac{1}{4}$	$\bar{x}, 0, \frac{1}{4}$	$0, x, \frac{1}{4}$	$0, \bar{x}, \frac{1}{4}$
			$\bar{x}, 0, \frac{3}{4}$	$x, 0, \frac{3}{4}$	$0, \bar{x}, \frac{3}{4}$	$0, x, \frac{3}{4}$

16	<i>i</i>	$\dots 2 \dots$	$x, x, \frac{1}{4}$	$\bar{x}, \bar{x}, \frac{1}{4}$	$\bar{x}, x, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$
			$\bar{x}, \bar{x}, \frac{3}{4}$	$x, x, \frac{3}{4}$	$x, \bar{x}, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$

8	<i>h</i>	$m \dots 2m$	$\bar{x}, x + \frac{1}{2}, 0$	$\bar{x}, \bar{x} + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, x, 0$	$x + \frac{1}{2}, \bar{x}, 0$
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8	<i>g</i>	$2 \dots mm$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z} + \frac{1}{2}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$
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8	<i>f</i>	$4 \dots$	$0, 0, z$	$0, 0, \bar{z} + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, z + \frac{1}{2}$
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8	<i>e</i>	$\dots 2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$
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4	<i>d</i>	$m \dots mm$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$		
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4	<i>c</i>	$4/m \dots$	$0, 0, 0$	$0, 0, \frac{1}{2}$		
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4	<i>b</i>	$\bar{4} 2m$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$		
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4	<i>a</i>	$4 2 2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$		
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