

## Precision Measurements of Lattice Parameters of Non-Cubic Crystals

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It is shown that lattice parameters of non-cubic crystals can be accurately determined by linear extrapolation against the function  $\frac{1}{2}(\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta)$  by selecting lines with suitable indices. Use can be made of the slope of the extrapolation curve of one of the parameters to derive the slope of the extrapolation curve of a second parameter. By this means, a true extrapolated value of the second parameter may be obtained when only a single appropriate reflexion is available. It is also shown that the observed  $\sin^2 \theta$  values can be accurately corrected for drift by means of an expression of the form  $D \sin^2 \theta (\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta)$ . Examples of lattice-parameter determinations and drift corrections are given for cobalt and for  $\text{Ni}_3\text{Ti}$ .

### Introduction

In a well-designed Debye-Scherrer camera free from specimen eccentricity, and using the film arrangement of Bradley & Jay (1932) which eliminates the effects of uniform film shrinkage, the only systematic errors in line-peak position which remain to be eliminated are those caused by the divergence of the X-ray beam from a finite focal spot and the absorption of the rays in the specimen. Taylor & Sinclair (1945) have shown that the peaks are displaced towards the higher angles by the amount

$$\Delta S = k(\cos \theta + \sin 2\theta / 2\theta), \quad (1)$$

where  $S$  is the distance between corresponding peaks on either side of the incident beam, and  $k$  is a constant dependent on the absorption factor of the specimen and on the shape and size of focal spot. It follows from (1) and the Bragg equation  $2a \sin \theta = n\lambda$  that the relative error in the spacing  $a$  computed from a single reflexion is

$$da/a = -(k/2R)(\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta). \quad (2)$$

Thus, if the value of  $a$  is computed for each measured value of  $\theta$  and the results plotted against

$$f(\theta) = \frac{1}{2}(\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta),$$

the plot should be perfectly linear over the whole range of angles from  $\theta = 0^\circ$  to  $\theta = 90^\circ$ , and the error in  $a$  should be zero at  $f(\theta) = 0$ . A practical demonstration of the linearity of  $f(\theta)$  in the case of cubic  $\text{Cu}_3\text{Al}_4$  has been given by Nelson & Riley (1945). It is obvious that the extrapolation method is quite general and may be applied directly to hexagonal, tetragonal and orthorhombic cells if spectra of the form  $h00$ ,  $0k0$  and  $00l$  are available. Since the slopes of these curves are proportional to the lattice parameters, it becomes possible to extrapolate to an accurate parameter from only a single reflexion, provided the slope of the extrapolation curve for at least one other parameter is known. A typical example is given in the next section for the case of cobalt.

### Extrapolation method for non-cubic crystals—cobalt

Cobalt can exist in two crystalline forms, face-centred cubic and close-packed hexagonal, but the stability of the two forms and the temperature at which the one transforms into the other are considerably influenced by crystal size, purity and degree of lattice distortion both prior and subsequent to its heat treatment (van Arkel, 1939, p. 327; Troiano & Tokich, 1948). Above about  $450^\circ\text{C}$ . the structure is face-centred cubic; below  $450^\circ\text{C}$ . it may completely transform to the hexagonal close-packed form, but most frequently it consists of an intimate mixture of the cubic and hexagonal forms, the latter displaying a 'mistakes' lattice (Edwards & Lipson, 1942*a, b*; Wilson, 1942).

Owing to the position of the cobalt absorption edge, the choice of radiations which give spectra with suitable indices at high Bragg angles for making accurate parameter determinations for cobalt is very limited. For the 100% cubic form, manganese radiation is ideal, since the 311 reflexion falls at  $79.93^\circ$  and the distance over which the extrapolation has to be made is very small. On the other hand, when the mixed form of cobalt is photographed the 311 reflexion is overlapped by 11 $\bar{2}$ 2 and appears somewhat diffuse, making accurate measurements difficult, and there are no suitable high-order hexagonal reflexions of the type  $hki0$  or  $000l$ . Using a 19 cm. diameter Debye-Scherrer camera and iron  $K\alpha$  radiation, it is possible clearly to resolve the  $\alpha$ -doublet of the cubic 222 reflexion from the hexagonal 0004 reflexion at the high Bragg angle of  $72^\circ$ . These reflexions are sufficiently strong to be measured with a high degree of precision, but quite the same degree of accuracy cannot be achieved for the weak 2020 reflexion at the Bragg angle of  $63^\circ$ , on which the  $a$  parameter depends.

In Fig. 1 are drawn the extrapolation curves for the cubic and hexagonal parameters. To obtain the

$c$  parameter of the hexagonal phase full use can only be made of 0004, since 0002 partly overlaps the cubic 111 reflexion, and it is impossible to measure its position accurately. Thus, to use the 0004 reflexion to full advantage, the  $c$  parameter is computed from it in the normal manner and an extrapolation curve drawn through the corresponding point having a slope  $c/a_w$  times the slope of curve  $a_w$  for the cubic phase. This is curve  $c$  in Fig. 1, the extrapolated value at  $f(\theta)=0$  being taken as the true value of the  $c$  parameter. The  $a$ -parameter extrapolation curve is given by the line through the points for 20 $\bar{2}$ 0 and 10 $\bar{1}$ 0. This has a slope  $a/a_w$  times the slope for curve  $a_w$ , which means that the position of the weak 20 $\bar{2}$ 0 reflexion has been determined with a high degree of accuracy and is yielding a satisfactory value for the  $a$  parameter.

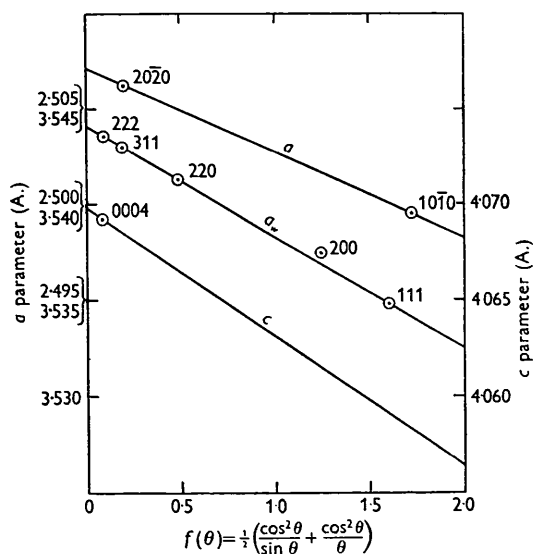


Fig. 1. Extrapolation curves for Hilger spectroscopically pure cobalt, annealed for 48 hr. at 400° C. and quenched. Fe K $\alpha$  radiation, 19 cm. diameter camera.

Values for the parameters in absolute Ångström units at 20° C., after correcting for refractive index (Weigle, 1934; Jette & Foote, 1935), are as follows:

$$\begin{aligned} \text{Cubic phase } a_w &= 3.5442 \text{ \AA.} \\ \text{Hexagonal phase } a &= 2.5074 \text{ \AA.} \\ c &= 4.0699 \text{ \AA.}, \\ c/a &= 1.62316. \end{aligned}$$

#### Calculation of 'drift' corrections for non-cubic crystals

For a powder pattern to be safely used as a means of phase identification, the positions and intensities of the lines must be accurately known in order to avoid confusion with possible reflexions from a second constituent. Unless the unit cell is extremely simple, the number of lines on the powder photograph will be quite large and, particularly in the higher orders where the  $\alpha$ -doublet is opening out, the pattern will be exceedingly complex. It may be possible to index the lower orders

by means of special charts (Hull & Davey, 1921; Bunn, 1945) for tetragonal or hexagonal crystals or to use the difference method, devised by Bradley & Taylor (1937) and extended by Lipson (1949), for orthorhombic crystals in which the unit cell is not too large, and, from the approximate parameters obtained thereby, to endeavour to index the higher orders of reflexion. The procedure then is to calculate rather more accurate parameters from the high-order reflexions and, from these, to compute a table of  $\sin^2\theta$  values which are compared with the observed values. The difference between observed and calculated values of  $\sin^2\theta$  is small for the high-order reflexions, since the parameter values are made to conform to them. It increases systematically as the Bragg angle decreases owing to the effects of absorption, and may change from 1 part in 80,000 above 70° to several parts in 1000 for reflexions below 45°. Thus, unless the observed  $\sin^2\theta$  values can be satisfactorily corrected for drift, it becomes difficult to decide to which reflexions the  $\sin^2\theta$ 's belong, and the risk of incorrect indexing through spurious agreements with the calculated values may be very great.

The displacement by absorption of the line peak towards a higher Bragg angle through the distance  $\Delta S$  produces a corresponding difference  $\Delta(\sin^2\theta)$  between the observed value of  $\sin^2\theta$  and the value computed from an accurate knowledge of the lattice parameters. Thus, to allow for drift, the Bragg equation should be written in the form

$$\begin{aligned} \sin^2\theta &= f(\lambda, a, b, c, h, k, l) + \Delta \sin^2\theta \\ &= f(\lambda, a, b, c, h, k, l) + D\phi(\theta), \end{aligned} \quad (3)$$

where  $D$  is a constant adjusted to give the best overall fit to the corrections, and  $\phi(\theta)$  is an expression which may be derived from the experimental conditions.

According to Hadding (1921), the peak is displaced by a distance  $\frac{1}{2}r(1 + \cos^2\theta)$  for the special case of an infinitely absorbing specimen of radius  $r$  and parallel radiation. This leads to a drift correction, for a camera of radius  $R$ , of the form

$$\begin{aligned} \Delta \sin^2\theta &= \sin 2\theta d\theta = \sin 2\theta r(1 + \cos 2\theta)/4R \\ &= (r \cos^2\theta \sin 2\theta)/2R; \end{aligned}$$

but since these theoretical conditions are never realized in practice, the expression is better written in the empirical form

$$\Delta \sin^2\theta = -D \cos^2\theta \sin 2\theta, \quad (4)$$

where the drift constant  $D$  is arbitrarily adjusted to suit the experimental conditions.

On the other hand, Cohen (1935) assumes from the extrapolation theory of Bradley & Jay that above  $\theta = 60^\circ$  the error in spacing takes the form

$$\Delta d/d \propto \cos^2\theta,$$

and therefore  $\Delta \sin^2\theta = -D \sin^2 2\theta$ . (5)

A closer examination of the Bradley-Jay discussion, which is based upon radiation diverging from a point

source upon an infinitely absorbing specimen, shows that in the absence of eccentricity

$$\Delta d/d = -\cot \theta d\theta = -(r \cos^2 \theta / 2\theta) (1/R + 1/AX), \quad (6)$$

where  $r$  is the radius of the specimen,  $R$  the radius of the camera, and  $AX$  the distance between the point focus at  $A$  and the specimen at  $X$ . Thus it follows that a more correct statement of the drift based upon the analysis of Bradley & Jay would be

$$\Delta \sin^2 \theta = -D \sin^2 2\theta / 2\theta. \quad (7)$$

This correction, however, does not take into account the effects of the intensity distribution in the focal spot and the incomplete absorption of the beam in the specimen. According to the detailed analysis of these factors by Taylor & Sinclair (1945 *a, b*), if  $\mu r > 1$ , where  $\mu$  is the linear absorption coefficient for the specimen of radius  $r$ , the line displacement is given to a high degree of accuracy by equation (1) and the lattice-parameter extrapolation function by equation (2). It therefore follows that the drift in  $\sin^2 \theta$  can be accurately expressed by an equation of the form

$$\Delta \sin^2 \theta = -D \sin^2 \theta (\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta). \quad (8)$$

In a sense, the application of the drift correction to the observed  $\sin^2 \theta$  values is equivalent to drawing an extrapolation curve, with the main difference that it is applicable to reflexions of the general type  $hkl$ , whereas the extrapolation curve is only directly applicable, for example, to reflexions of the type  $h00$ ,  $0k0$ ,  $00l$  for orthorhombic crystals. Cohen (1935), in his method of determining parameters by least squares, makes drift corrections of the general type and uses the corrected values of  $\sin^2 \theta$  to set up a series of difference equations from which the correct values of the lattice parameters are obtained. This method, in addition to being tedious, has the disadvantage of placing equal emphasis on strong reflexions which are accurately measurable and weak reflexions which may be subject to serious error. The extrapolation method, on the other hand, is simple to apply and has the marked advantage of pictorial representation, which instantly reveals errors in measurement or calculation. The drift correction is best applied to obtaining good agreement between observed and calculated  $\sin^2 \theta$  values in order to make certain of the correct indexing of spectra of the general type, and to act as a check on the accuracy of the parameters determined by the method of extrapolation.

#### Calculation of the lattice parameters of $\text{Ni}_3\text{Ti}$ and correction of $\sin^2 \theta$ values for drift

According to Laves & Wallbaum (1939),  $\text{Ni}_3\text{Ti}$  is a hexagonal close-packed structure with lattice parameters (scaled from  $kX$ . to  $\text{A}$ .) of  $a = 2.553$ ,  $c = 8.321$   $\text{A}$ .,  $c/a = 3.259$  and with 4 atoms in the unit cell. Weissenberg patterns revealed very faint superlattice lines which required a doubling of the  $a$  parameter, but these lines were not visible on the powder photograph taken with copper  $K\alpha$  radiation in a 57.3 mm. diameter Debye-

Scherrer camera, using  $\text{NaCl}$  as a calibrating substance. Reflexions in the powder pattern up to a Bragg angle of only  $45^\circ$  were measured, and the parameters derived from them were averaged so that the accuracy of the determinations fell below that normally achieved by making use of high-angle reflexions.

In the present investigation, parameters with an accuracy of at least 1 part in 30,000, to check variability in composition, were required, and every individual line had to be accounted for in order to identify any possible impurities. Since, from a calculation of the  $\sin^2 \theta$  values based on the structure of Laves & Wallbaum, it was found that the 0008 reflexion would appear at about  $70^\circ$  when iron  $K\alpha$  radiation was employed, it was decided to obtain the  $c$  parameter from an iron-radiation

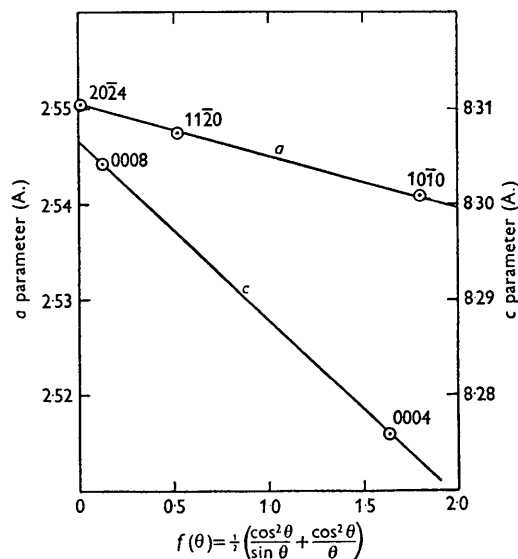


Fig. 2. Extrapolation curves for  $\text{Ni}_3\text{Ti}$ .  $\text{Fe } K\alpha$  radiation, 9 cm. diameter camera.

pattern using the 0008 and 0004 reflexions at  $68.93$  and  $27.9^\circ$  respectively, to give the necessary linear extrapolation curve against the function

$$\frac{1}{2}(\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta).$$

The slope of this curve was used to ensure that the extrapolation curve for the  $a$  parameter, based on the  $11\bar{2}0$  and  $10\bar{1}0$  reflexions at  $49.5$  and  $26.1^\circ$  respectively, was satisfactory. These curves are shown in Fig. 2. As an additional check, the value of  $a$  from the  $20\bar{2}4$  reflexion at  $83.15^\circ$  was computed using a drift-adjusted value for  $\sin^2 \theta_{0004}$ , and this was found to lie accurately on the  $a$ -extrapolation curve shown in Fig. 2. Correcting for refractivity, the lattice parameters at  $20^\circ\text{C}$ . for  $\text{Ni}_3\text{Ti}$  were found to be

$$\begin{aligned} a &= 2.5505 \text{ A.}, \\ c &= 8.3067 \text{ A.}, \\ c/a &= 3.2569. \end{aligned}$$

Using these accurately determined lattice parameters from the relatively simple iron-radiation photograph,

the  $\sin^2 \theta$  values for copper  $K\alpha$  radiation were computed and compared with values obtained from a pattern of  $\text{Ni}_3\text{Ti}$  taken with copper radiation in the 19 cm. diameter Debye-Scherrer camera. In this way, the lines of the much more complex copper-radiation photograph could be indexed with reasonable certainty, and fresh extrapolation curves could be drawn for the  $hki0$  and  $000l$  reflexions, as shown in Fig. 3. The lattice parameters so obtained agreed with the values obtained with iron radiation. As a check on the indexing of the lines, and in particular those of the form  $hkil$ , a drift correction was applied to all the  $\sin^2 \theta$  values.

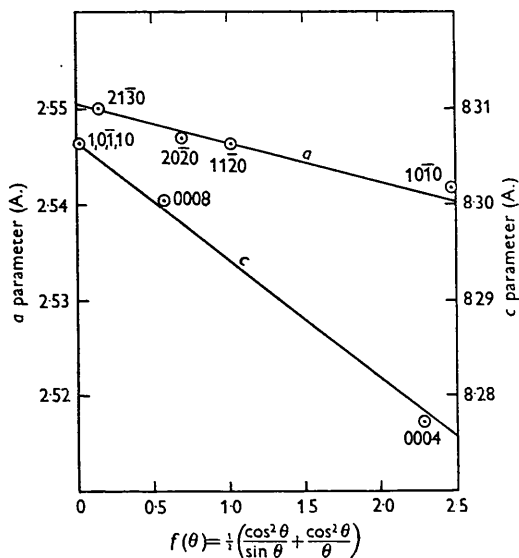


Fig. 3. Extrapolation curves for  $\text{Ni}_3\text{Ti}$ .  $\text{Cu } K\alpha$  radiation, 19 cm. diameter camera.

To apply the drift correction, the values of the difference,  $\Delta \sin^2 \theta$ , between observed and calculated  $\sin^2 \theta$ 's for all reflexions were obtained and used to compute a best value of  $D$  in the expression

$$\Delta \sin^2 \theta = -D \sin^2 \theta (\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta).$$

Using this best value of the drift constant, the appropriate theoretical correction was applied to all the observed  $\sin^2 \theta$ 's. It is evident from the 4th, 5th and 6th columns of Table 1, that the correlation between the drift-corrected observed and the calculated  $\sin^2 \theta$  values is satisfactory over the whole angular range, the major differences being due to errors in measuring the film and to a trace of residual nickel primary solid solution.

For comparison purposes, the Cohen and Hadding corrections, using the most favourable value of the drift constant for each, are also given in the table. It is evident that both corrections go violently astray, but in opposite directions at the lower angles. In addition to these, a column giving the correction factor based on a reinterpretation of the Bradley-Jay analysis of line position is also given. The last-named differs very little from that based on the more detailed analysis of line

shape given by Taylor & Sinclair, which is rather surprising considering the radical difference in treatment.

In order to bring out the difference between the various expressions for the drift correction, the functions are plotted in Fig. 4. Only the function

$$\frac{1}{2} \sin^2 \theta (\cos^2 \theta / \sin \theta + \cos^2 \theta / \theta)$$

has been drawn on a natural scale, the other functions being on a scale which gave the best fit between observed and calculated values of  $\sin^2 \theta$  in the case of  $\text{Ni}_3\text{Ti}$ . The unsuitability of the Cohen and Hadding

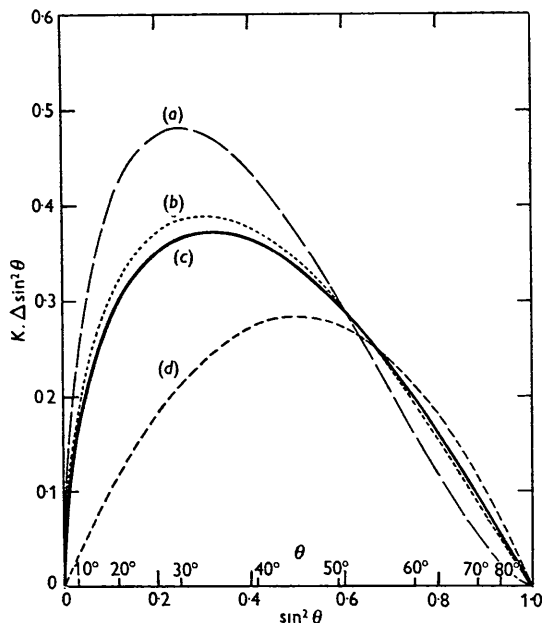


Fig. 4.  $\sin^2 \theta$  drift correction curves. Values of  $\Delta \sin^2 \theta$ :

- (a) Hadding,  $D \cos^2 \theta \sin 2\theta$ ;
- (b) Bradley-Jay,  $D \frac{\sin^2 2\theta}{2\theta}$ ;
- (c) Taylor-Floyd,  $D \sin^2 \theta \left[ \frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta} \right]$ ;
- (d) Cohen,  $D \sin^2 2\theta$ .

corrections becomes apparent from these curves, and would have appeared even more pronounced if a camera of smaller radius had been employed.

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Table 1.  $\sin^2\theta$  data for  $\text{Ni}_3\text{Ti}$ 

Copper  $K\alpha$  radiation; 19 cm. diameter Debye-Scherrer camera. Extrapolated values corrected for refractivity.  $a=2.5505$ ,  $c=8.3067$  A.;  $c/a=3.2569$ .

Intensity	$hkl$	$\sin^2\theta$			(Calc. $\sin^2\theta$ - corr. $\sin^2\theta$ ) $\times 100,000$				
		Obs.	Corr. (Taylor & Floyd)	Calc.	Taylor & Floyd	Cohen	Hadding	Bradley & Jay	
<i>m</i>	10 $\bar{1}$ 0	0.12266	0.12168	0.12181	13	-46	52	19	
<i>s</i>	10 $\bar{1}$ 1	0.13146	0.13047	0.13043	-4	-62	36	3	
<i>s</i>	0004	0.13879	0.13779	0.13781	3	-55	43	6	
<i>vs</i>	10 $\bar{1}$ 2	0.15752	0.15647	0.15626	-21	-78	22	-15	
<i>s</i>	10 $\bar{1}$ 3	0.20050	0.19939	0.19933	-6	-59	34	1	
<i>m</i>	10 $\bar{1}$ 4	0.26085	0.25968	0.25962	-6	-54	30	0	
<i>m</i>	10 $\bar{1}$ 5	0.33935	0.33716	0.33713	-3	-41	26	1	
<i>ms</i>	11 $\bar{2}$ 0	0.36660	0.36542	0.36544	2	-32	28	6	
<i>ms</i>	10 $\bar{1}$ 6	0.43295	0.43181	0.43187	6	-19	25	9	
<i>vvw</i>	20 $\bar{2}$ 0	0.48858	0.48750	0.48725	-25	-43	-12	-22	
<i>w</i>	20 $\bar{2}$ 1	0.49645	0.49538	0.49587	49	-32	61	52	
<i>m</i>	11 $\bar{2}$ 4	0.50430	0.50324	0.50324	0	-16	11	2	
<i>w-m</i>	20 $\bar{2}$ 2	0.52293	0.52189	0.52170	-19	-33	-10	-17	
<i>w-m</i>	10 $\bar{1}$ 7	0.54432	0.54331	0.54384	53	42	60	55	
<i>w-m</i>	0008	0.55203	0.55103	0.55122	19	8	25	20	
<i>w</i>	20 $\bar{2}$ 3	0.56537	0.56439	0.56477	38	31	42	39	
<i>vw</i>	20 $\bar{2}$ 4	0.62543	0.62455	0.62506	51	38	50	51	
<i>vw</i>	10 $\bar{1}$ 8	$\alpha_1$	0.67244	0.67165	0.67192	27	27	21	27
		$\alpha_2$	0.67562	0.67483	0.67527	44	44	38	43
<i>w</i>	20 $\bar{2}$ 5	$\alpha_1$	0.70193	0.70120	0.70141	21	23	13	20
		$\alpha_2$	0.70575	0.70503	0.70491	-12	-9	-20	-13
<i>m</i>	20 $\bar{2}$ 6	$\alpha_1$	0.79686	0.79634	0.79599	-35	-28	-49	-37
		$\alpha_2$	0.80081	0.80030	0.79997	-33	-26	-47	-35
<i>w-m</i>	10 $\bar{1}$ 9	$\alpha_1$	0.81820	0.81773	0.81809	36	43	23	34
		$\alpha_2$	0.82269	0.82223	0.82218	-5	5	-20	-7
<i>vvw</i>	21 $\bar{3}$ 0	$\alpha_1$	0.85155	0.85116	0.85128	12	18	-2	9
		$\alpha_2$				Not measured			
<i>w-m</i>	21 $\bar{3}$ 1	$\alpha_1$	0.86014	0.85977	0.85987	10	16	-2	7
		$\alpha_2$	0.86444	0.86408	0.86417	9	16	-5	6
<i>ms</i>	*21 $\bar{3}$ 2	$\alpha_1$	0.88626	0.88596	0.88567	-29	-22	-42	-31
		$\alpha_2$	0.89115	0.89086	0.89010	-76	-70	-89	-79
<i>w</i>	20 $\bar{2}$ 7	$\alpha_1$	0.90793	0.90769	0.90777	8	14	-4	6
		$\alpha_2$	0.91279	0.91256	0.91231	-25	-19	-37	-28
<i>m-s</i>	11 $\bar{2}$ 8	$\alpha_1$	0.91558	0.91536	0.91514	-22	-16	11	-24
		$\alpha_2$	0.92053	0.92032	0.91971	-61	-56	-72	-63
<i>w-m</i>	21 $\bar{3}$ 3	$\alpha_1$	0.92887	0.92868	0.92866	-2	3	-13	-4
		$\alpha_2$	0.93355	0.93338	0.93331	-7	-2	-17	-9
		$\alpha_1$	0.98147	0.98142	0.98146	4	6	0	3
		$\alpha_2$	0.98642	0.98639	0.98637	-2	0	-4	-2

\* Overlaps the 331 reflexion from the trace of cubic nickel-rich phase which is present.