LA-2317
PHYSICS AND MATHEMATICS
(TID-4500, 14th Ed.)

LOS ALAMOS SCIENTIFIC LABORATORY
OF THE UNIVERSITY OF CALIFORNIA LOS ALAMOS NEW MEXICO

REPORT WRITTEN: April 1959

REPORT DISTRIBUTED: September 3, 1959

**A MATHEMATICAL TECHNIQUE FOR THE
PRECISION DETERMINATION OF LATTICE CONSTANTS**

by

Richard E. Vogel and Charles P. Kempter

This report expresses the opinions of the author or
authors and does not necessarily reflect the opinions
or views of the Los Alamos Scientific Laboratory.

Contract W-7405-ENG. 36 with the U. S. Atomic Energy Commission

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ABSTRACT

An IBM 704 code has been developed for the precision determination of crystal lattice constants, using the Hess method as a basis with the following modifications:

1. No approximations are made in the solution of the observation equation.
2. The method is extended to the hexagonal and orthorhombic crystal systems.
3. The method is extended to include the diffractometer.
4. The method is extended to additional extrapolation functions for the Debye-Scherrer technique.

It was concluded that the Hess method is an excellent approximation for the case which he treated (i.e., that the errors in Φ are directly proportional to Φ for $\Phi \leq 60^\circ$, where Φ is twice the complement of the Bragg angle). In other cases treated, with randomly selected materials, the Hess approximation gave excellent results as compared to the exact technique; however, because of certain restrictions the exact technique is recommended.

ACKNOWLEDGMENT

The authors wish to express their thanks to R. K. Zeigler and R. H. Moore for their constructive criticisms and helpful suggestions, and to F. H. Ellinger and J. M. Leitnaker for the loan of the beta tin and ZrB_2 (I) films, respectively. Also they are indebted to M. R. Nadler for the preparation of the lithium wire.

CONTENTS

	Page
Abstract	3
Acknowledgment	5
Introduction	9
Mathematical Treatment	14
Results and Discussion	24
References	28

FIGURES

Fig. 1. Case 1A	22
Fig. 2. Case 1B	22
Fig. 3. Case 2	22
Fig. 4. Case 3	23
Fig. 5. Case 4	23

TABLE

Table I	29
-------------------	----

INTRODUCTION

The precision determination of crystal lattice constants is a powerful technique for basic studies of the solid state. Examples include the precise measurement of bond distances, true densities, thermal expansions, compressibilities, and solid solution effects.

Graphical extrapolation methods for the elimination of systematic errors in lattice constant measurements have been treated by many investigators. Their correct usage has been discussed by Cooper, Jordan, and Kempter,¹ and the most useful extrapolation functions tabulated as a function of Bragg angle.

Analytical methods have been discussed by Cohen² and Hess.³ These methods are more readily applicable to noncubic crystal systems than extrapolation methods, but the complexity of the calculations necessitates the use of a computing machine. Of the two analytical methods, the Hess method is certainly preferable since it assigns statistical weights to the observed points. This weighting is a necessity since the weighting function increases tremendously as the Bragg angle approaches $90^\circ \theta$.

For the cubic system, using a Debye-Scherrer or symmetrical back reflection focusing camera, Hess started his fitting procedure with the following general equation expressing the function F.

$$F = A_0 \alpha + K_0 \delta - \gamma \quad (1)$$

where $A_0 = 1/a_0^2$; a_0 = the lattice constant

$$\alpha = \frac{1}{2} \lambda^2 n^2 (h^2 + k^2 + \ell^2); \quad \lambda = \text{wave length}$$

n = an integer

hkl = Miller indices

K_0 = the "drift constant"

$\delta = \Phi \sin \Phi$, the error term, which assumes

$$\Delta \Phi \propto \Phi, \text{ where } \Phi = \pi - 2\theta$$

$$\gamma = 1 + \cos \Phi = 2 \sin^2 \theta$$

By setting K_0 equal to zero, Hess calculated values of F_0 at every observed point and also arrived at the weighting function $\csc^2 \Phi$.

Using Deming's⁴ method, he solved for A_0 and K_0 and then for a_0 . Hess also treated the tetragonal lattice and the flat-film symmetrical back reflection camera.

The following general equations apply for the crystal systems treated in this report, where a_0 , b_0 , and c_0 are lattice constants and

δ is the error term, which will be discussed later. See Equation 1 for the definitions of λ , hkl , K_0 , and γ . The integer n is omitted since it is equal to unity.

$$\text{Cubic} \quad F = A_0 \alpha + K_0 \delta - \gamma \quad (2)$$

$$\text{where} \quad A_0 = 1/a_0^2 ; \quad \alpha = \frac{1}{2} \lambda^2 (h^2 + k^2 + \ell^2)$$

$$\text{Tetragonal} \quad F = A_0 \alpha + B_0 \beta + K_0 \delta - \gamma \quad (3)$$

$$\text{where} \quad A_0 = 1/a_0^2 ; \quad B_0 = 1/c_0^2$$

$$\alpha = \frac{1}{2} \lambda^2 (h^2 + k^2) ; \quad \beta = \frac{1}{2} \lambda^2 \ell^2$$

$$\text{Hexagonal} \quad F = A_0 \alpha + B_0 \beta + K_0 \delta - \gamma \quad (4)$$

$$\text{where} \quad A_0 = 4/3 a_0^2 ; \quad B_0 = 1/c_0^2$$

$$\alpha = \frac{1}{2} \lambda^2 (h^2 + hk + k^2) ; \quad \beta = \frac{1}{2} \lambda^2 \ell^2$$

$$\text{Orthorhombic} \quad F = A_0 \alpha + B_0 \beta + C_0 \epsilon + K_0 \delta - \gamma \quad (5)$$

$$\text{where} \quad A_0 = 1/a_0^2 ; \quad B_0 = 1/b_0^2 ; \quad C_0 = 1/c_0^2$$

$$\alpha = \frac{1}{2} \lambda^2 h^2 ; \quad \beta = \frac{1}{2} \lambda^2 k^2 ; \quad \epsilon = \frac{1}{2} \lambda^2 \ell^2$$

The error term δ is selected according to the measurement geometry and the experimental techniques used.¹ By definition $\delta = \Delta \Phi \sin \Phi / K_0$, where $\Phi = (\pi - 2\theta)$.

For the symmetrical back reflection focusing camera, the systematic errors in $\Delta a_0/a_0$ are proportional to $\phi \tan \phi$, where $\phi = (90^\circ - \theta) = \frac{1}{2} \Phi$.

Therefore, $\delta = K_0 \Phi \sin \Phi / K_0 = \Phi \sin \Phi$. In terms of ring diameter, s , and camera diameter, D ,

$$\delta = \frac{s}{2D} \sin \frac{s}{2D} \quad (6)$$

For the Debye-Scherrer camera, the systematic errors in $\Delta a_0/a_0$ are proportional to $\phi \tan \phi$, $\cos^2 \theta$, or $\frac{1}{2}(\frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta})$ depending upon the experimental techniques used. Therefore,

$$\delta = \Phi \sin \Phi, \sin^2 2\theta, \text{ or } \sin^2 2\theta \left(\frac{1}{\sin \theta} + \frac{1}{\theta} \right), \text{ respectively.}$$

In terms of s and D these become:

$$\delta = \frac{s}{D} \sin \frac{s}{D} \quad (7)$$

$$\delta = \sin^2 \left(\pi - \frac{s}{D} \right) \quad (8)$$

$$\delta = \sin^2 \left(\pi - \frac{s}{D} \right) \left[\frac{1}{\sin \left(\frac{\pi}{2} - \frac{s}{2D} \right)} + \frac{1}{\left(\frac{\pi}{2} - \frac{s}{2D} \right)} \right] \quad (9)$$

For the diffractometer, the systematic errors in $\Delta a_0/a_0$ caused by displacement of the specimen surface from focusing circle are proportional to $\cos \theta \cot \theta$. Therefore, $\delta = \sin \theta \cos^2 \theta$. Since 2θ is the measurement made in this method, the final equation becomes:

$$\delta = \sin \frac{2\theta}{2} \cos^2 \frac{2\theta}{2} \quad (10)$$

Other error terms may of course be substituted and/or additional error terms added by solving for $\Delta \Phi$ and then for δ . The angles in equations 6 through 9 are in radians.

No attempt was made to extend the code to the monoclinic and triclinic crystal systems because of their limited usefulness; the rhombohedral system may of course be indexed on hexagonal axes.

In the IBM 704 code the crystal systems in Equations 2, 3, 4, and 5 are referred to as problems 1, 2, 3, and 4, respectively; the error terms in equations 6, 7, 8, 9, and 10 are referred to as cases 1A, 1B, 2, 3, and 4, respectively.

MATHEMATICAL TREATMENT

The problem is to determine estimates of the parameters for Equations 2, 3, 4, and 5. A general equation, which includes 2, 3, 4, and 5, can be written:

$$y_e = \sum_{i=1}^m a_i x_{ie} \quad (11)$$

where

$$y_e = \gamma_e$$

$$x_{1e} = \alpha_e$$

$$x_{2e} = \delta_e$$

$$x_{3e} = \beta_e$$

$$x_{4e} = \epsilon_e$$

$$a_1 = A_0$$

$$a_2 = K_0$$

$$a_3 = B_0$$

$$a_4 = C_0$$

$e = 1, \dots, N$; N = number of experimental data points and $m = 2$ for the cubic system, $m = 3$ for the tetragonal and hexagonal systems, and $m = 4$ for the orthorhombic. The variables y_e and x_{2e} are both functions of θ .

Estimates of the parameters can be obtained from the experimental data by the method of least squares. Minimizing the function

$$Q = \sum_{e=1}^N w_e F_e^2 \quad (12)$$

where

$$F_e = \sum_{i=1}^m a_i x_{ie} - y_e$$

w_e = the weight associated with each F_e

will give the weighted least square estimate of the parameters.

Previous work³ has indicated that the variance of y given x is not constant, hence a weighting function w_e should be used and appears in Equation 12. By the method of Maximum Likelihood (Ref. 5, pp. 551-552), the weighting function w_e can be shown to be inversely proportional to the variance $\sigma_{F_e}^2$ of F_e . Since F_e is a function of θ_e , we may write by the Theory of Error Propagation

$$\sigma_{F_e}^2 = \left(\frac{\partial F_e}{\partial \theta_e} \right)^2 \sigma_{\theta_e}^2$$

The random error of θ_e is assumed constant* and acts as a proportionality constant which can be ignored in the analysis, thus

$$\sigma_{F_e}^2 = \left(\frac{\partial F_e}{\partial \theta_e} \right)^2 = \left(\sum_{i=1}^m \frac{\partial x_{ie}}{\partial \theta_e} a_i - \frac{\partial y_e}{\partial \theta_e} \right)^2$$

and

$$w_e = 1 / \left(\sum_{i=1}^m \frac{\partial x_{ie}}{\partial \theta_e} a_i - \frac{\partial y_e}{\partial \theta_e} \right)^2$$

The weighting function for Equations 6, 7, 8, 9, and 10 are given respectively by Equations 13, 14, 15, 16, and 17.

* The reading of a large number of diffraction films have shown this assumption to be valid.

$$w_e = \frac{1}{4 \left[K_0 (\pi - \theta) \cos 2\theta - (K_0 + 1) \sin 2\theta \right]^2} \quad (13)$$

$$w_e = \frac{1}{\left[- (K_0 + \frac{1}{2}) \sin (\frac{90^\circ - \theta}{2}) - K_0 (\frac{\frac{\pi}{2} - \theta}{2}) \cos (\frac{90^\circ - \theta}{2}) \right]^2} \quad (14)$$

$$w_e = \frac{1}{4 \left[K_0 \sin 4\theta - \sin 2\theta \right]^2} \quad (15)$$

$$w_e = \frac{1}{\left\{ K_0 \left[4 \cos^3 \theta - 8 \sin^2 \theta \cos \theta + \frac{2 \sin 4\theta}{\theta} - \frac{\sin^2 2\theta}{\theta^2} \right] - 2 \sin 2\theta \right\}^2} \quad (16)$$

$$w_e = \frac{1}{\left[K_0 \cos \theta (\cos^2 \theta - 2 \sin^2 \theta) - 2 \sin 2\theta \right]^2} \quad (17)$$

where $\theta = \frac{\pi}{2} - \frac{\Phi}{2}$, $\Phi = \frac{s_e}{D}$ radians, except for Equation 15,

where $\Phi = \frac{s_e}{2D}$.

Because w_e is a function of the parameters, an iterative method⁴ is used to minimize Q. Let us redefine Q to be

$$Q = \sum_{e=1}^N w_e \left(\sum_{i=1}^m (a_{0i} - \Delta a_{0i}) x_{ie} - y_e \right)^2 \quad (18)$$

where a_{0i} is an approximation for a_i and $\Delta a_{0i} = a_i - a_{0i}$.

Combining terms we get

$$Q = \sum_{e=1}^N w_e \left(F_e - \sum_{i=1}^m \Delta a_{0i} x_{ie} \right)^2 \quad (19)$$

Taking the partial derivative of Equation 19 with respect to the parameters and equating them to zero yields the following normal equations

$$\Delta a_{01} \sum_{e=1}^N w_e x_{1e}^2 + \Delta a_{02} \sum_{e=1}^N w_e x_{1e} x_{2e} + \cdots = \sum_{e=1}^N w_e x_{1e} F_e$$

$$\Delta a_{01} \sum_{e=1}^N w_e x_{1e} x_{2e} + \Delta a_{02} \sum_{e=1}^N w_e x_{2e}^2 + \cdots = \sum_{e=1}^N w_e x_{2e} F_e$$

$$\begin{matrix} \cdot & \cdot \\ \cdot & \cdot \end{matrix}$$

$$\Delta a_{01} \sum_{e=1}^N w_e x_{1e} x_{me} + \Delta a_{02} \sum_{e=1}^N w_e x_{1e} x_{2e} + \cdots =$$

$$\sum_{e=1}^N w_e x_{me} F_e$$

Let the matrix $||\Delta a_{0i}|| = ||\Delta a_{01} \Delta a_{02} \cdots \Delta a_{0m}||$,

$$\text{the matrix } ||x_{ij}|| = \begin{vmatrix} \sum w_e x_{le}^2 & \cdots & \sum w_e x_{le} x_{me} \\ \vdots & & \vdots \\ \sum w_e x_{le} x_{me} & \cdots & \sum w_e x_{me}^2 \end{vmatrix}$$

$$\text{and the matrix } ||F_j|| = \begin{vmatrix} \sum w_e x_{le} F_e \\ \vdots \\ \sum w_e x_{me} F_e \end{vmatrix}$$

The normal equations then become

$$||\Delta a_{0i}|| \cdot ||x_{ij}|| = ||F_j||$$

$$\text{and } ||\Delta a_{0i}|| = ||F_j|| \cdot ||x_{ij}||^{-1}$$

From the solution of the $||\Delta a_{0i}||$ matrix we are then able to improve our approximation for the parameters in Equation 12 by applying the formula

$$a'_i = a_{0i} - \Delta a_{0i}$$

where a'_i becomes the new approximation a_{0i} in Equation 18. With this new approximation the entire process is repeated. This iteration procedure is continued until the correction parameters Δa_{0i} are deemed "sufficiently small."

Estimates of the standard deviations of the parameters can be shown to be

$$S.D. a_i = \sqrt{\frac{Q_F}{N-m}} \cdot x_{ii}^{-1}$$

where Q_F = the value of Q obtained from the last iteration and x_{ii}^{-1} is the ii element of the inverse matrix $||x_{ij}||^{-1}$. The standard deviation of the parameter(s) is used in determining confidence limits for the parameter(s) and also in testing to see if the parameters are significantly different from zero (Ref. 5, p. 540).

It should be pointed out that stopping after the first iteration as Hess³ has suggested is not theoretically sufficient when computing the standard deviation of the parameters. Although K_0 values are quite small, it has been shown that there exist some K_0 's which are statistically significantly different from zero. Hence, using zero as the approximation for K_0 will not always give the statistically best estimate of the $||x_{ij}||^{-1}$ matrix, which one uses in the computation of the standard deviation. It is recommended that if one uses such

an approximation, i.e., setting K_0 equal to zero and stopping after the first iteration, the $\|x_{ij}\|^{-1}$ matrix and the Q function should be computed with the new approximations before computing the standard deviation of the parameters.

A useful subjective technique to determine the "reasonableness" of the fit is to order the y observed values and compare them to the y's which have been calculated from the x's and the fitted parameters. By forming y observed minus y calculated, and examining the signs of these differences, one can imply the fit is reasonable if the signs are randomly distributed.

Although the iterative technique should be carried out until convergence is reached when using high speed computers, it is of interest to those who do not have such facilities to evaluate an approximation technique for determining lattice constants. Using K_0 equal to zero and approximations for the lattice constants good to three digits and stopping after the first iteration gave excellent approximations for the lattice constants of the materials we tested. Just how well this approximation does compared to the convergent iterative technique is a function of K_0 and the range of θ used.

Since the weighting function is a function of K_0 , choosing K_0 equal to zero removes terms in the weighting function, cf. Equations 13 through 17. Weights were calculated for K_0 equal to zero and K_0 fairly large and their percent differences were plotted (see Figures 1 through 5). If the percent difference over the range of θ used is

constant, then the two weighting functions differ by most a multiplicative factor which does not affect the final computations. It is virtually impossible to compute what value of K_0 and what range of θ will give significantly poor estimates of the lattice constants by using this approximation, thus Figures 1 through 5 are to be used subjectively by the experimenter to decide whether he feels a single iteration is sufficient.

RESULTS AND DISCUSSION

The results for a number of representative examples of the problems and cases run are tabulated in Table I in order of increasing mass absorption coefficients (μ_m in cm^2/g). The cubic, tetragonal, hexagonal, and orthorhombic crystal systems are designated as problems 1, 2, 3, and 4 respectively; the error equations 6, 7, 8, 9, and 10 are designated as cases 1A, 1B, 2, 3, and 4 respectively. K_0 is the "drift constant" and a_0 , b_0 , and c_0 are the lattice constants in Angstrom units at 25°C ; σ is the precision of the parameter expressed as the standard deviation.

Each example was computed by two methods. The first, designated by AP, was an approximate technique, i.e., setting K_0 equal to zero and stopping after the first iteration. The standard deviation of the parameters were computed with the first $\|x_{ij}\|^{-1}$ matrix and the correct Q function. The second method, designated by EX, was an exact technique, i.e., continuous iteration until convergence was reached.

International Union of Crystallography standard specimens are designated I.U.C. Copper radiation (nickel filtered) was used in all cases, except for Li and UC, where cobalt radiation (iron filtered) and chromium radiation (vanadium filtered) were used, respectively. The lattice constants are not corrected for refraction. Lonsdale's⁶ 1950 wavelengths were used in all computations. All specimens, except Li in the form of wire, were -325 mesh and were not diluted. Debye-Scherrer specimens were run in 0.3 mm diameter Lindemann glass capillaries; back reflection specimens were run on rubber cement-coated cardboard. Case 1A films

were read by three readers, thus tripling the number of points. For numbers 20, 21, and 22, only very high Bragg angle reflections were measured. For cases 2 and 3, a film should properly be corrected for film shrinkage;¹ in order to show the effect of this correction, the film for number 21 has been corrected for shrinkage. The film for beryllium is unique in that the shrinkage correction factor is unity. The lattice constant obtained for number 7 has been corrected only for the specimen surface displacement error.

It was noted that for all of the Debye-Scherrer films examined, the absolute value of K_0 was highest for case 2, lowest for case 3, and intermediate for case 1B. It can be readily shown that K_0 is actually an analytical systematic errors constant which is related to the extrapolation systematic errors constant K'' by a simple relationship. Using the cubic system and case 1 as an example: The error equation is $\Delta a_0/a_0 = K' \phi \tan \phi$, where $\phi = (\pi/2 - \theta)$ radians. In practice, values of the lattice constant are plotted against corresponding values of $\phi \tan \phi$ and a linear extrapolation is carried out to $\phi \tan \phi = 0$. Therefore, $a = K'' \phi \tan \phi + a_0$, where K'' is the slope and a_0 is the y-intercept. Substituting Δa_0 for $(a - a_0)$ and dividing the equation by a_0 , we obtain:

$$\frac{\Delta a_0}{a_0} = \frac{K''}{a_0} \phi \tan \phi, \text{ and } K' = K''/a_0$$

By differentiation of the Bragg equation:

$$\frac{\Delta a_0}{a_0} = - \cot \theta \Delta \theta = - \tan \phi \Delta \phi$$

And since $K_0 = \Delta \Phi / \Phi = \Delta \phi / \phi$, and so $\Delta \phi = K_0 \phi$:

$$\frac{\Delta a_0}{a_0} = - K_0 \phi \tan \phi = K' \phi \tan \phi$$

$$\therefore K_0 = - K' = - K''/a_0$$

Similarly it can be shown that $K' = K''/a_0$ for all cases, and that $K_0 = - K''/2a_0$, $- K''/4a_0$, and $- 2K''/a_0$ for cases 2,3, and 4 respectively.

Since many factors¹ influence the systematic errors constant, it is very difficult to predict its value. Reference to Table I shows that a prediction cannot be made on the assumption that absorption is the overriding cause of systematic error.

An examination of Table I shows that, in general, the Hess method is an excellent approximation for the lattice constants and K_0 values for the problems and cases treated. All of the lattice constants are rounded off at the sixth decimal place. [It is standard practice to round off precision lattice constants to five decimal places (since the wavelengths used have five decimal places) after the refraction correction has been added on.] It should be noted that as the absolute value of K_0 increases, the approximate lattice constants diverge from the exact values; the a_0 and c_0 values for number 8

illustrate this divergence. The divergence also increases as the Bragg angle range increases, as pointed out in the mathematical discussion. Thus, in using the approximate method, one must also be selective in choosing the Bragg angle range. Cases 1 and 2 are properly applied to reflections greater than 57° and $60^\circ \theta$, respectively; however, cases 3 and 4 have wide ranges of applicability.¹ All of the Bragg angles used in the preparation of Table I were back reflection angles.

Further examination of Table I illustrates the approximate method of computing standard deviations, i.e., using the first $|| x_{ij} ||^{-1}$ matrix obtained, is very good. It should be noted again that as the absolute value of K_0 increases, the approximation to the standard deviation of the parameters becomes poor (see number 8). It must be remembered that approximations made in this manner are only estimates for the standard deviations computed exactly, hence smaller standard deviations obtained by the approximation technique compared to the iterative convergence technique does not imply that one gets smaller errors on the lattice constants by using the approximation technique.

It is concluded that, in general, a single iterative technique (such as the Hess method), is an excellent approximation; however, in view of certain restrictions, a convergent iterative technique is recommended. The advantage of the latter technique is that it yields the best estimate of the lattice constant(s) and the standard

deviation(s), regardless of the error function used.

All computations in Table I were done with an IBM 704 Fortran code written by one of the authors (R. E. Vogel).

REFERENCES

1. Dorothy L. Cooper, Thomas L. Jordan, Jr., and Charles P. Kempter, Los Alamos Scientific Laboratory Report LA-2308, March, 1959.
2. M. U. Cohen, Rev. Sci. Instr. 6, 68 (1935) and 7, 155 (1936); Z. Krist. 94A, 288, 306 (1936).
3. James B. Hess, Acta Cryst. 4, 209 (1951).
4. W. E. Deming, "Statistical Adjustment of Data," John Wiley & Sons, Inc., New York, 1943.
5. A. Hald, "Statistical Theory with Engineering Applications," John Wiley & Sons, Inc., New York, 1952.
6. K. Lonsdale, Acta Cryst. 3, 400 (1950).

TABLE I

No.	Problem	Case	Material	μ_m	No. Pts.	K_0	σ_{K_0}	a_0	σ_{a_0}	b_0	σ_{b_0}	c_0	σ_{c_0}
1AP 1EX	1 1	1B 1B	Li	1.13 1.13	3 3	-0.000587 -0.000587	0.000373 0.000373	3.509553 3.509553	0.000173 0.000173				
2AP 2EX	1 1	1A 1A	I.U.C. Diamond	5.5	12 12	-0.002803 -0.002803	0.000089 0.000089	3.567145 3.567145	0.000061 0.000061				
3AP 3EX	1 1	1A 1A	I.U.C. Silicon	60.3	18 18	-0.002832 -0.002832	0.000106 0.000106	5.430482 5.430482	0.000055 0.000055				
4AP 4EX	1 1	1B 1B	I.U.C. Silicon	60.3	18 18	0.000795 0.000795	0.000172 0.000172	5.430502 5.430502	0.000089 0.000089				
5AP 5EX	1 1	2 2	I.U.C. Silicon	60.3	18 18	0.000935 0.000934	0.000196 0.000196	5.430527 5.430527	0.000091 0.000091				
6AP 6EX	1 1	3 3	I.U.C. Silicon	60.3	18 18	0.000454 0.000454	0.000098 0.000098	5.430498 5.430498	0.000088 0.000088				
7AP 7EX	1 1	4 4	Norelco Std. Silicon	60.3	4 4	-0.001083 -0.001083	0.001382 0.001382	5.429923 5.429923	0.000484 0.000484				
8AP 8EX	3 3	2 2	ZrB ₂ I	116	15 15	0.011948 0.011961	0.004668 0.004674	3.169989 3.169995	0.001477 0.001491			3.531080 3.531066	0.003796 0.003824
9AP 9EX	3 3	3 3	ZrB ₂ I	116	15 15	0.005728 0.005728	0.002199 0.002199	3.169898 3.169899	0.001456 0.001458			3.530827 3.530824	0.003727 0.003731
10AP 10EX	3 3	1B 1B	ZrB ₂ II	116	19 19	0.002361 0.002361	0.000118 0.000118	3.169227 3.169227	0.000065 0.000065			3.530773 3.530773	0.000160 0.000160
11AP 11EX	3 3	2 2	ZrB ₂ II	116	19 19	0.003133 0.003133	0.000160 0.000160	3.169261 3.169261	0.000067 0.000067			3.530910 3.530910	0.000165 0.000165
12AP 12EX	3 3	3 3	ZrB ₂ II	116	19 19	0.001360 0.001360	0.000068 0.000068	3.169223 3.169223	0.000065 0.000065			3.530771 3.530771	0.000160 0.000160
13AP 13EX	3 3	1A 1A	ZrB ₂ II	116	30 30	-0.004501 -0.004501	0.000107 0.000107	3.169092 3.169092	0.000011 0.000011			3.530891 3.530891	0.000058 0.000058
14AP 14EX	3 3	1B 1B	NbB ₂	125	6 6	0.002265 0.002266	0.001157 0.001156	3.101700 3.101700	0.001782 0.001782			3.293083 3.293083	0.000180 0.000180
15AP 15EX	3 3	2 2	NbB ₂	125	6 6	0.003823 0.003825	0.002077 0.002074	3.102673 3.102675	0.002491 0.002487			3.293201 3.293201	0.000201 0.000201
16AP 16EX	1 1	1A 1A	I.U.C. Tungsten	171	9 9	-0.002830 -0.002830	0.000095 0.000095	3.165073 3.165073	0.000037 0.000037				
17AP 17EX	4 4	1A 1A	Yellow HgO	207	8 8	-0.003073 -0.003073	0.000627 0.000628	6.610087 6.610087	0.000304 0.000304	5.519638 5.519638	0.001479 0.001479	3.520338 3.520337	0.000439 0.000439

TABLE I (continued)

[illegible]