sistently prepared. The standard deviation of six crystals was approximately ±0·012 p.p.m. One crystal of PERFX was measured by X-ray and optical interferometry (Deslattes & Henins, 1973) to give $d_{2\bar{2}0}$ (25 °C) = 1·9201715 Å ± 0·30 p.p.m. and this was later confirmed as 1·9201718 Å ± 0·25 p.p.m. (Deslattes *et al.*, 1974) but altered to 1·9201706 Å ± 0·15 p.p.m. (Deslattes, Henins, Schoonover & Carroll, 1976) following the correction of a systematic error. Under vacuum the Bragg spacing is 0·34 p.p.m. larger. Since this precision is far below the reproducibility of PERFX and is comparable with the range of lattice parameters measured in Table 1 for float-zoned silicon, it would seem that any source of such silicon could be used to access the absolute value of lattice spacing. IR absorption measurements can be used to measure the carbon concentration and the necessary correction is (Baker *et al.*, 1968) $\Delta d/d = -6{\cdot}5 \times 10^{-24} n_{\rm C}$ where $n_{\rm C}$ is the number of carbon atoms per cm^3.

At a rather lower precision one can have access to the PERFX lattice parameter by using Czochralski-grown oxygen-contaminated silicon. After IR determination of the oxygen concentration the lattice-parameter shift can be calculated from $\Delta d/d = +3{\cdot}8 \times 10^{-24} n_{\rm O}$ where $n_{\rm O}$ is the number of oxygen atoms per cm^3.

Within the errors of measurement all of the values in the right-hand column of Table 1 are therefore effectively on the absolute scale.

Hubbard, Swanson & Mauer (1975) have recently announced that a large quantity of powdered float-zoned silicon has been made available for calibration purposes in powder diffractometry. Since they were only concerned with *reproducibility* to 10 p.p.m. and not with absolute lattice spacings, it seems that the important attribute of this proposed standard is not the manifestly well defined lattice parameter of the starting material but the ill defined quality of the resultant powder. The wording of their recommendation that one uses 'the powder diffraction value of 5·430880 Å for the *lattice parameter* of the Standard Reference Material silicon' is amazing. The lattice parameter of Deslattes *et al.* (1976) for PERFX was 5·43106446 Å ± 0·15 p.p.m. in vacuum.

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Absorption-Weighted Mean Path Lengths for Spheres

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Accurate values (~0·05%) of the absorption-weighted mean path lengths for spheres as a function of μR and θ have been calculated by differentiation of the table of values of absorption corrections [Dwiggins (1975). *Acta Cryst.* A**31**, 395–396].

Introduction

The absorption-weighted mean path length, $\bar{T}$, needed in extinction corrections, has been calculated for spheres from the approximate formula (Coppens & Hamilton, 1970)

$$\bar{T}=\frac{\ln A^*}{\mu},$$

where A^* is the absorption correction factor and μ the linear absorption coefficient. This expression, however, is inappropriate for $\mu R > 0{\cdot}25$ (Becker & Coppens, 1974). The correct formula is

$$\bar{T}=\frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}\mu},$$

but there are no tabulated values of the derivative, $\mathrm{d}A^*/\mathrm{d}\mu$, available. With absorption corrections of high precision, such as those given by Dwiggins (1975), it is possible to calculate the derivative from the table of A^* values.

Method

We may write

$$\bar{T}=\frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}\mu}=R\left[\frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}(\mu R)}\right],$$

where R is the radius of the sphere. The absorption corrections for a sphere are given in a table of A^* values as a function of μR and θ, $[\mu R = 0, 0{\cdot}1, 0{\cdot}2\ldots, \theta = 0{\cdot}, 5{\cdot}, 10{\cdot}, \ldots, 90{\cdot}]$, where θ is the Bragg angle of a reflection.

To calculate the value of $\mathrm{d}A^*/\mathrm{d}(\mu R)$ at one of the points of this grid, we fix a fourth-order polynomial through the points ($\mu R \pm 0{\cdot}2$, $\mu R \pm 0{\cdot}1$, μR; θ) and determine the derivative at (μR,θ). The equations are given in the Appendix. This method is clearly not applicable for the points on the grid with $\mu R = 0$ and $\mu R = 0{\cdot}1$ since no values exist for A^* at $\mu R = -0{\cdot}2$ and $-0{\cdot}1$.

For $\mu R = 0$, we know that $A^* = 1$ and $\bar{T} = \frac{3}{2}R$ for a sphere. Hence

$$\left[\frac{1}{A^*}\frac{\mathrm{d}A^*}{\mathrm{d}(\mu R)}\right]_{\mu R=0}=\frac{3}{2}.$$

For the points at $\mu R = 0{\cdot}1$, we have chosen to fix a fourth-order polynomial passing through ($\mu R = 0{\cdot}, 0{\cdot}1, 0{\cdot}2, 0{\cdot}3$; θ) and with $[\mathrm{d}A^*/\mathrm{d}(\mu R)]_{\mu R=0} = \frac{3}{2}$. The equations are given in the Appendix. We prefer to keep the results in the form of $(1/A^*)(\mathrm{d}A^*/\mathrm{d}\mu R)$ as a two-dimensional function of θ and μR rather than $\bar{T}$ as a three-dimensional function of θ, μ and R. We have implemented this method in a Fortran program

Table 1. *Values of* $(1/A^*)(\mathrm{d}A^*/\mathrm{d}\mu R)$ *for spheres*

TH = θ°, MUR = μR.

MUR	TH= 0	TH= 5	TH=10	TH=15	TH=20	TH=25	TH=30	TH=35	TH=40	TH=45	TH=50	TH=55	TH=60	TH=65	TH=70	TH=75	TH=80	TH=85	TH=90
.0	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000
.1	1.4845	1.4842	1.4829	1.4809	1.4782	1.4739	1.4690	1.4634	1.4569	1.4504	1.4439	1.4375	1.4309	1.4248	1.4191	1.4152	1.4117	1.4096	1.4089
.2	1.4692	1.4682	1.4650	1.4611	1.4548	1.4472	1.4374	1.4268	1.4145	1.4019	1.3879	1.3748	1.3615	1.3491	1.3385	1.3292	1.3228	1.3180	1.3168
.3	1.4527	1.4515	1.4476	1.4400	1.4309	1.4186	1.4044	1.3886	1.3708	1.3517	1.3327	1.3128	1.2947	1.2773	1.2624	1.2494	1.2397	1.2340	1.2321
.4	1.4360	1.4341	1.4283	1.4190	1.4058	1.3898	1.3709	1.3492	1.3265	1.3018	1.2773	1.2531	1.2296	1.2089	1.1903	1.1748	1.1628	1.1560	1.1533
.5	1.4166	1.4161	1.4090	1.3969	1.3803	1.3598	1.3360	1.3093	1.2812	1.2522	1.2231	1.1946	1.1678	1.1434	1.1218	1.1044	1.0910	1.0825	1.0797
.6	1.4011	1.3980	1.3890	1.3742	1.3538	1.3289	1.3006	1.2693	1.2365	1.2033	1.1700	1.1382	1.1087	1.0816	1.0577	1.0383	1.0239	1.0147	1.0115
.7	1.3830	1.3792	1.3683	1.3507	1.3264	1.2973	1.2643	1.2286	1.1918	1.1549	1.1164	1.0839	1.0516	1.0225	.9978	.9767	.9615	.9518	.9484
.8	1.3641	1.3600	1.3473	1.3262	1.2984	1.2650	1.2275	1.1879	1.1473	1.1071	1.0684	1.0314	.9976	.9674	.9409	.9195	.9034	.8931	.8898
.9	1.3451	1.3401	1.3253	1.3013	1.2696	1.2321	1.1908	1.1474	1.1038	1.0608	1.0198	.9815	.9465	.9152	.8880	.8663	.8495	.8391	.8359
1.0	1.3255	1.3198	1.3029	1.2758	1.2401	1.1987	1.1535	1.1070	1.0608	1.0157	.9733	.9340	.8978	.8661	.8392	.8167	.8001	.7897	.7859
1.1	1.3058	1.2993	1.2800	1.2497	1.2103	1.1651	1.1165	1.0670	1.0185	.9720	.9266	.8886	.8522	.8205	.7931	.7709	.7542	.7437	.7400
1.2	1.2851	1.2780	1.2566	1.2228	1.1799	1.1312	1.0796	1.0278	.9777	.9299	.8858	.8455	.8093	.7776	.7506	.7285	.7120	.7017	.6981
1.3	1.2645	1.2563	1.2324	1.1961	1.1494	1.0967	1.0430	.9892	.9377	.8895	.8451	.8048	.7691	.7378	.7113	.6895	.6733	.6631	.6596
1.4	1.2449	1.2349	1.2090	1.1684	1.1180	1.0628	1.0068	.9517	.8990	.8504	.8064	.7666	.7315	.7009	.6749	.6539	.6377	.6278	.6243
1.5	1.2231	1.2133	1.1845	1.1398	1.0867	1.0295	.9711	.9145	.8615	.8133	.7696	.7308	.6964	.6665	.6414	.6209	.6055	.5957	.5922
1.6	1.2015	1.1908	1.1585	1.1118	1.0555	.9957	.9358	.8782	.8261	.7778	.7350	.6970	.6638	.6349	.6105	.5907	.5758	.5663	.5628
1.7	1.1806	1.1681	1.1339	1.0836	1.0244	.9621	.9005	.8435	.7912	.7444	.7027	.6659	.6334	.6057	.5822	.5632	.5484	.5394	.5361
1.8	1.1586	1.1456	1.1087	1.0558	.9939	.9294	.8669	.8101	.7579	.7121	.6711	.6359	.6053	.5787	.5561	.5376	.5236	.5148	.5117
1.9	1.1370	1.1226	1.0835	1.0275	.9625	.8964	.8341	.7774	.7262	.6817	.6420	.6078	.5791	.5535	.5321	.5144	.5010	.4924	.4892
2.0	1.1152	1.0996	1.0584	.9982	.9318	.8646	.8019	.7457	.6962	.6527	.6160	.5830	.5550	.5305	.5098	.4927	.4799	.4717	.4687
2.1	1.0932	1.0772	1.0327	.9703	.9014	.8340	.7712	.7157	.6678	.6259	.5899	.5588	.5322	.5088	.4886	.4726	.4603	.4523	.4494
2.2	1.0719	1.0543	1.0074	.9427	.8719	.8039	.7421	.6874	.6402	.6003	.5658	.5353	.5098	.4884	.4699	.4548	.4426	.4347	.4311
2.3	1.0498	1.0316	.9822	.9150	.8434	.7744	.7133	.6605	.6147	.5758	.5433	.5141	.4896	.4692	.4518	.4363	.4252	.4175	.4149
2.4	1.0275	1.0118	.9583	.8889	.8147	.7462	.6870	.6340	.5918	.5507	.5212	.4937	.4699	.4500	.4328	.4187	.4076	.4003	.3986
2.5	1.0108	.9691	.9297	.8562	.7904	.7074/	.6554	.6194	.5618	.5589	.4980	.4776	.4554	.4315	.4142	.4028	.3921	.3883	.3783

SPHCOR. The A^* data for μR from 0·0 to 2·5 are taken from Dwiggins (1975) and the values of $(1/A^*)(dA^*/d\mu R)$ are given in Table 1. $\bar{T}$ values are retrieved by multiplying $(1/A^*)(dA^*/d\mu R)$ by R at the appropriate values of μR and θ.

The accuracy of the table of A^* values (Dwiggins, 1975) is claimed to be 0·05%. We have compared the values of A^* of Dwiggins and $\bar{T}$ calculated by the present method with values given by a Gaussian-grid integration program of unknown accuracy obtained from Cromer (1977). For example, for a value of μR = 1·0 we find relative discrepancies in the A^* values of 0·06% ($\theta = 0°$) and 0·1% ($\theta = 90°$), whereas those in the $\bar{T}$ values are 0·03% ($\theta = 0°$) and 0·05% ($\theta = 90°$). We conclude that the accuracy of our $\bar{T}$ table is about 0·05%.

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APPENDIX

1. We desire the derivative dy/dx at $x = 0$ for a fourth-order polynomial passing through the points

$$(-2x,y_{2-})\,(-x,y_-)\,(0,y_0)\,(x,y_+)\,(2x,y_{2+}).$$

Thus we fix

$$y = Ax^4 + Bx^3 + Cx^2 + Dx + E \qquad (1)$$

and

$$\frac{dy}{dx} = 4Ax^3 + 3Bx^2 + 2Cx + D$$

$$\left(\frac{dy}{dx}\right)_{x=0} = D$$

Substituting for the values of the points in (1), we obtain

$$\begin{aligned}
y_{2-} &= 16Ax^4 - 8Bx^3 + 4Cx^2 - 2Dx + E\\
y_- &= Ax^4 - Bx^3 + Cx^2 - Dx + E\\
y_0 &= E\\
y_+ &= Ax^4 + Bx^3 + Cx^2 + Dx + E\\
y_{2+} &= 16Ax^4 + 8Bx^3 + 4Cx^2 + 2Dx + E.
\end{aligned}$$

Solving for D, we find

$$D = \left(\frac{dy}{dx}\right)_{x=0} = \frac{y_{2-} - 8y_- + 8y_+ - y_{2+}}{12x}.$$

2. We desire $(dy/dx)_{x=0}$ for a fourth-order polynomial (1) passing through the points $(-x,y_-)(0,y_0)(x,y_+)$-$(2x,y_{2+})$ and having $(dy/dx)_{-x} = 1\cdot5$. Thus we obtain

$$\begin{aligned}
y_- &= Ax^4 - Bx^3 + Cx^2 - Dx + E\\
y_0 &= E\\
y_+ &= Ax^4 + Bx^3 + Cx^2 + Dx + E\\
y_{2+} &= 16Ax^4 + 8Bx^3 + 4Cx^2 + 2Dx + E\\
1.5 &= -4Ax^3 + 3Bx^2 - 2Cx + D.
\end{aligned}$$

Solving for D we find

$$D = \left(\frac{dy}{dx}\right)_{x=0} = \frac{1}{18x}(-17y_- + 9y_0 + 9y_+ - y_{2+} - 9x).$$

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The Crystal Structure of Ganophyllite, a Complex Manganese Aluminosilicate.
I. Polytypism and Structural Variation

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The reciprocal-lattice geometry of ganophyllite has been investigated by X-ray diffraction, two distinct variants being noted. These structures, comprising a monoclinic form and a hitherto unreported triclinic variant, can both be interpreted in terms of structural columns which can be stacked in varying sequences along either of the {011} planes. Diffracted intensities from models of this type for both variants give good agreement with the distinctive pattern of intensities actually observed. With the structural column concept, it is also possible to explain instances of two-dimensionally disordered intergrowths of these structures.