pounds; however, in five cases ordering could not be determined even if it existed. We note that the patterns all have high symmetry $(F\overline{4}3m)$ for zincblende and $P6_{1}mc$ for wurtzite related compounds). Ordering of the cations seems rather unlikely. The composition 12_236_4 is located on the connecting line between 26 and 136₂. Examples are known where a complete series of solid solutions exists between 26 and 136_2 . Goryunova (1965) lists for example CdTe-AgInTe₂ and CdTe-CuInTe₂ where the zincblende structure type is found over the entire concentration range. The compositions CuCd₂InTe₄ and AgCd₂InTe₄ given in Table 7 are, therefore, only selected points of a complete series of solid solutions. For the other compounds given in Table 7 no homogeneity range measurements have been made, and it must be left for further research to determine if these alloys really correspond to independent quaternary compounds or to the quaternary compositions in a solid solution range between a binary and a ternary normal tetrahedral structure compound.

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Eine neue Absorptionsfaktortafel für kugelförmige Proben

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A new table of spherical absorption factors is calculated for $0 \le \mu R \le 31.5$ with an accuracy better than 10^{-3} . Errors up to 2% are detected in the absorption factor tables 5.3.6B of *International Tables for X-ray Crystallography*, Vol.II.

Überblick

Das Integral A_{Kug} zur Berechnung von Kugelabsorptionsfaktoren ist, wenn man von den Beugungswinkeln $\theta = 0^{\circ}$ und $\theta = 90^{\circ}$ absieht, nicht geschlossen darstellbar (Bond, 1957); es muss daher numerisch bestimmt werden.

Die ersten Berechnungen von A_{Kug} -Werten findet man bei Taylor (1944). Er setzte die Kugel nach Fig.1 aus Kreisscheibchen abnehmenden Halbmessers r zusammen, wodurch sich das Kalkül auf eine eindimensionale Integration über die bereits bekannten Absorptionsfaktoren A_{Zy1} des Kreiszylinders (Claasen, 1930; Bradley, 1935) reduzieren lässt.

Unter Berücksichtigung der Volumennormierung findet man für eine Scheibchendicke Δz

$$A_{\rm Kug} \simeq \Sigma r^2 \pi A_{\rm Zyl}(\mu r) \Delta z / (4\pi R^3/3) , \qquad (1)$$

wobei, wie üblich, R für den Kugelradius und μ für den linearen Schwächungskoeffizienten gesetzt ist. Für

 $\Delta z \rightarrow 0$ geht die Summe (1) in das Integral (2) über (Taylor, 1944):

$$A_{\rm Kug} = \frac{3}{4} \int_{-1}^{+1} (r/R)^2 A_{\rm Zyl}(\mu r) d(z/R) \,. \tag{2}$$

Die wenigen Taylorschen Integralwerte wurden von Evans & Ekstein (1952) erstmals durch eine systematische Tabelle ersetzt. Die Autoren benutzten jedoch die wenig handliche Summation (1), weshalb sie den mit μR wachsenden Einfluss der Kugelrandzone dadurch berücksichtigten, dass sie eine von z abhängige Scheibendicke Δz einführten.

Jene erste Tabelle hat Bond (1957, 1959) durch eine ausführlichere, direkt über das Volumenintegral berechnete, ersetzt. Trotz elektronischer Rechenhilfsmittel war eine hinreichend genaue numerische Integration so zeitaufwendig, dass sich Bond auf die Berechnung einiger weniger Stützpunkte im Abstand $\theta = (15 \cdot n)^{\circ}$ (n = 1, ...6) beschränken und die Zwischengebiete interpolieren musste. Die Bondsche Tabelle umfasst den Bereich $\mu R \le 10$. Mittlerweile neu berechnete Azyl-Werte (Weber, 1967) versetzten uns in die Lage, mit Hilfe einer Integration (2) die Genauigkeit der interpolierten A_{Kug} -Werte an allen Tafelpunkten direkt zu überprüfen. Es zeigte sich, dass die von Bond benutzte Interpolationsfunktion die Absorptionswerte zwar im Bereich $\theta > 15^{\circ}$ innerhalb der Tafelstellenzahl richtig wiedergibt, dass sie aber für $0 < \theta$ $< 15^{\circ}$, dem Gebiet der stärksten Änderung von $A_{\rm Kug}$, Fehler bis zu 2% liefert.

Die gute Konvergenz des hier benutzten Verfahrens erlaubte es, die Tafel unter Wahrung einer Genauigkeitsgrenze von 10^{-3} , bis $\mu R = 31,5$ auszudehnen.

Die numerische Integration und die Abschätzung ihrer Genauigkeit

Definiert man, wie in Fig. 1 eingetragen, einen Winkel α durch

$$z/R = \sin \alpha , \qquad (3)$$



Fig. 1. Approximation der Kugel durch kreiszylindr. Scheibchen nach Taylor. r = Scheibchenradius, R = Kugelradius, P = Primärstrahlrichtung.

so gilt $r/R = \cos \alpha$ und $dz/R = \cos \alpha d\alpha$. Mit diesen Substitutionen geht der Ausdruck (2) in das mit der Simpsonregel numerisch gut auswertbare Integral (4) über.

$$A_{\rm Kug} = \frac{3}{2} \int_0^{\mu/2} \cos^3 \alpha A_{\rm Zyl}(\mu R \cos \alpha) d\alpha \,. \tag{4}$$

Die Fig.2(*a*) und (*b*) zeigen das Konvergenzverhalten von Gl.(4) an den Tabellenrändern $\theta = 0^{\circ}$ und $\theta = 90^{\circ}$. Die wahren Integrationsfehler $|\Delta I|$ liessen sich durch Einsetzen fehlerfreier A_{Zy1} -Werte in Gl.(4) und Vergleich mit direkt berechneten A_{Kug} einfach gewinnen.

Für $\theta \neq 0^{\circ}$ oder 90° stehen hinreichend genaue Näherungswerte A_{Zy1} über die Gl.(5) zur Verfügung.

$$A_{\rm Zy1} \simeq A_{\rm MBT9}(\theta) = \sum_{k} \int g_k(l) \exp\left(-\mu l\right) dl .$$
 (5)

Diese Gleichung findet man im Rahmen eines früher angegebenen, dort mit MBT9 bezeichneten Verfahrens diskutiert [Weber, 1967, Gln. (5) und (6)]. Der grösste relative Fehler $|\Delta A_{Zyl}/A_{Zyl}|$ liegt mit 7. 10⁻⁴ bei $\theta = 5^{\circ}$ und $\mu r \simeq 1.6$ (r=Zylinderradius); bei $\theta = 10^{\circ}$ überschreiten die A_{Zyl} -Fehler den Betrag von 3. 10⁻⁴ nicht mehr, sinken mit zunehmendem θ weiter ab, durchlaufen ein breites Minimum und nähern sich erst wieder bei $\theta = 90^{\circ}$ und $\mu r = 30$ einem Betrag von 4. 10⁻⁴. Der Einfluss dieser Fehler auf Gl. (4) ist aus Fig. 2(c)zu ersehen. Da die Weglängenverteilungsfunktionen $g_{\theta}(l)$ für die θ -Ränder $\theta_G = 0^\circ$ und 90° extrem sind und die $\theta \neq \theta_G$ die Funktionen $g_{\theta}(l)$ in die der beiden Ränder stetig überführen, darf die für die Ränder bewiesene Konvergenz auch für das Tabelleninnere als gesichert gelten. Einen numerischen Beweis für $\mu R \le 10$ liefert die Tabelle 1.

Tabelle 1. Abweichungen in % zwischen direkt über das Volumenintegral berechneten A_{Kug}-Werten (Tabelle 5.3.6A der International Tables for X-ray Crystallography(1959) Bd. 2 S. 300) und den Integrationsergebnissen nach Gl. (4)

$\mu R/\theta$	15°	30°	45°	60°	75°
0,5	0,01	0,00	0,00	0,02	0,00
1	0,02	0,00	0,00	0,02	0,00
2	0,06	-0,03	0,01	0,01	0,02
3	0,03	0,04	0,01	0,04	0,02
4	0,01	0,04	0,02	0,03	0,03
5	0,02	0,03	0,04	0,04	0,04
6	0,04	0,01	0,05	0,08	0,05
7	0,06	-0,02	0,02	0,04	0,15
8	0,11	-0,05	0,04	0,05	0,04
9	0,09	-0,11	0,03	0,07	0,02
10	0.13	-0.13	-0.03	1.64	0.01

Ergebnisse

Die Berechnung der neuen Tafel (Tabelle 2) beruht auf der Integration (4) unter Anwendung der Simpsonregel, wobei eine Intervallteilung $d\alpha$ von $\pi/200$ für $\mu R \le 9$ und von $\pi/400$ für $\mu R > 9$ benutzt ist. Damit bleibt der Tafelfehler für alle A_{Kug} mit Sicherheit unter 10⁻³. In Tabelle 1 sind die von Bond über das Volumenintegral berechneten Tafelstützpunkte (Tabelle 5.3.6A, International Tables for X-ray Crystallography, 1959) mit hier gewonnenen Integralwerten verglichen. Mit wenigen Ausnahmen liegen die Abweichungen unter 10^{-3} . An der Stelle $\mu R = 10$, $\theta = 60^{\circ}$ hat sich in die

Tabelle 2. Absorptionskorrekturfaktoren $A^* = 1/A_{Kug}$ für kugelförmige Proben

| μR | 8=0° | 5° | 10 ⁰
 | 15 ⁰ | 20 [°] | 2 5 ⁰
 | 30° | 35 ⁰ | 40 ⁰
 | 4 5 ⁰ | 50 [°] | 55 ⁰ | 60 ⁰
 | 65 ⁰ | 70 ⁰ | 75 ⁰
 | 80 ⁰ | 85 ⁰ | 90 ⁰
 | μR |
---	---	--
---	--	---
--	--	---
--	---	---
---	--	--
--	--	---
0.0	1.000 1.161	1.000 1.161
 | 1.000
1.161 | 1.000
1.161 | 1.000
1.160
 | 1.000
1.160 | 1.000
1.160 | 1.000
 | 1.000 | 1.000 | 1.000 | 1.000
 | 1.000 | 1.000
1.157 | 1.000
 | 1.000 | 1.000 | 1.000
 | 0.0 |
| .2 | 1.346 | 1.346 | 1.345
 | 1.345 | 1.344 | 1.343
 | 1.342 | 1.340 | 1.338
 | 1.337 | 1.335 | 1.333 | 1.331
 | 1.330
1.516 | 1.328 | 1.327
 | 1.326 | 1.325 | 1.325
 | .2
.3 |
| .4 | 2.076 | 1.799 | 2.071
 | 2.065 | 2.057 | 2.046
 | 2.034 | 2.020 | 2.006
 | 1.752 | 1.742 | 1.734 | 1.725
 | 1.717 | 1.710 | 1.704
 | 1.700 | 1.697 | 1.696
 | .4
.5 |
| .6
.7 | 2,390
2,747 | 2.389 | 2.382
 | 2.372 | 2.358 | 2.341
 | 2,320 2.638 | 2.298 | 2.275
 | 2.250
2.532 | 2.226
2.495 | 2.202
2.460 | 2.179
2.427
 | 2.159
2.398 | 2.141
2.372 | 2.126
2.351
 | 2.115 2.335 | 2.108 | 2.106
 | .6
.7 |
| .8
.9 | 3.151
3.608 | 3.147
3.603 | 3.131
3.579
 | 3.107
3.543 | 3.074 | 3.034 3.438
 | 2.988
3.372 | 2,939
3,303 | 2.887 3.231
 | 2.835
3.159 | 2.784
3.090 | 2.735
3.024 | 2.689
2.964
 | 2.648
2.910 | 2.613
2.863 | 2.585
2.825
 | 2.563
2.798 | 2.550
2.780 | 2.545
2.774
 | .8
.9 |
| 1.0
.1 | 4.124
4.704 | 4.115
4.691 | 4.082
4.644
 | 4.031
4.573 | 3.963
4.479 | 3.882
4.369
 | 3.792
4.248 | 3.697
4.122 | 3.600
3.995
 | 3.505
3.871 | 3.413
3.754 | 3.328
3.645 | 3.250
3.547
 | 3.180
3.460 | 3.121
3.386 | 3.073
3.327
 | 3.038
3.283 | 3.016
3.256 | 3.008
 | 1.0
.1 |
| .2 | 5.355 | 5.337 | 5.273
 | 5.175 | 5.048 | 4.901
 | 4.741 | 4.577 | 4.414
 | 4.257 | 4.110 | 3.975
4.317 | 3.854
4.170
 | 3.747
4.042 | 3.658 | 3.586
3.849
 | 3.532
3.786 | 3.500
3.747 | 3.488
3.734
 | .2
.3 |
| .4 | 7.802 | 7.755 | 7.605
 | 6.373
7.377 | 7.093 | 6.776
 | 6.447 | 6.124 | 5.815
 | 5.087 | 4.867 | 4.670
5.033 | 4.495
 | 4.344 | 4.217 | 4.117
 | 4.042 | 3.997 | 3.981
4.231
 | .4
.5 |
| .7 | 8.807
9.921 | 8.746 9.841 | 8.550
9.589
 | 8.257 9.215 | 7.895 | 7.498
 | 7.092 | 6.698 | 6.326
 | 5.985 | 5.678
6.101 | 5.405
5.787 | 5.168
5.514
 | 4.965
5.283 | 4.796
5.091 | 4.662
4.939
 | 4.564 | 4.504
4.760 | 4.483
4.736
 | .6
.7 |
| .8
.9 | 11.15 | 11.05 | 10.73
 | 10.26 | 9.690 | 9.089
 | 9.246 | 8.583 | 7.982
 | 6.946
7.447 | 6.535
6.979 | 6.176
6.572 | 5.867
6.224
 | 5.605
5.931 | 5.389
5.691 | 5.219
 | 5.094
5.362 | 5.018
5.277 | 4.991
5.248
 | .8
.9 |
| 2.0 | 14.00
15.64 | 13.83 | 13.32
 | 12.60 | 11.75 | 10.87
 | 10.03 | 9.262 | 8.570
 | 7.961
8.487 | 7.432
7.893 | 6.975
7.385 | 6.587
6.955
 | 6.262
6.595 | 5.995
6.301 | 5.785
6.071
 | 5.632
5.902 | 5.537
5.799 | 5.505
5.763
 | 2.0
.1 |
| .2 | 17.42 | 17.16 | 16.38
 | 15.29 | 14.07 | 12.85
 | 12.59 | 11.44 | 10.43
 | 9.023 | 8,362 | 7.800 | 7.326
 | 6.931 | 6.610 | 6.358
 | 6.174 | 6.061 | 6.022
 | .2 |
| .5 | 23.80 | 23.30 | 21.92
 | 20.05 | 18.05 | 16.14
 | 14.45 | 12.98 | 11.74
 | 10.69 | 9.810 | 9.074 | 8.461
 | 7.956 | 7.547 | 7.228
 | 6.996 | 6.852 | 6.803
 | .4 |
| .0 | 28.99 | 25.69 | 24.03
 | 23.69 | 21.01 | 18.55
 | 16.41 | 14.60 | 13.09
 | 11.26 | 10.30 | 9.507 | 9.233
 | 8.302 | 7.863 | 7.520
 | 7.271 | 7.117 | 7.064
 | .6 |
| .9 | 35.02 | 33.98 | 31.21
 | 27.71 | 24.21 | 21.10
 | 18.46 | 16.28 | 14.49
 | 13.02 | 11.82 | 10.83 | 10.01
 | 9.351 | 8.818 | 8.403
 | 8.102 | 7.915 | 7.850
 | .9 |
| 3.0 | 38.38 | 37.14 | 33.90
 | 29.86 | 25.90 | 22.42
 | 19.52 | 17.14
18.01
18.89 | 15.20
 | 13.62 | 12.33 | 11.27 | 10.41
 | 9.704 | 9.139 | 8.699
 | 8.379 | 8.181 | 8.113
 | 3.0 |
| .3 | 49.91 | 47.90 | 42.84
 | 36.85 | 31.27 | 26.58
 | 22.80 | 19.79 | 17.38
 | 15.45 | 13.37 | 12.63 | 11.60
 | 10.41 | 9.783 | 9.293
 | 9.216 | 8.716 | 8.639
 | -3 |
| .5 | 58.91 | 56.19 | 49.54
 | 41.93 | 35.09 | 29.50
 | 25.07 | 21.60 | 18.86
 | 16.69 | 14.95 | 13.54 | 12.40
 | 11.49 | 10.76 | 10.19
 | 9.776 | 9.519 | 9.430
 | .5 |
| .6 | 63.83 | 65.43 | 53.12
56.84
 | 44.60 | 37.07 | 30.99
 | 26.23 | 22.52 | 20.37
 | 17.31 | 15.48 | 14.00 | 12.81
 | 11.85 | 11.08 | 10.49
 | 10.06 | 9.787 | 9.693
 | .6
.7 |
| .9 | 80.38 | 75.65 | 64.72
 | 53.06 | 43.24 | 35.60
 | 29.78 | 25.34 | 21.90
 | 19.21 | 17.08 | 15.39 | 14.02
 | 12.93 | 12.06 | 11.39
 | 10.82 | 10.32 | 10.22
 | .8 |
| 4.0 | 86.52 | 81.14
86.89 | 68.87
73.17
77 61
 | 56.03
59.07 | 45.37 | 37.18
38.77
40.39
 | 30.99 | 26.29 | 22.67
 | 19.85 | 17.63 | 15.85 | 14.43
 | 13.29 | 12.39 | 11.69
 | 11.18 | 10.86 | 10.75
 | 4.0 |
| .3 | 106.9 | 99.15
105.7 | 82.19
 | 65.34 | 51.97 | 42.02
 | 34.67 | 29.18 | 25.00
 | 21.78 | 19.26 | 17.26 | 15.66
 | 14.02 | 13.05 | 12.29
 | 12.03 | 11.40 | 11.28
 | .2 |
| .5 | 122.3 | 112.5 | 91.74
 | 71.86 | 56.52 | 45.32
 | 37.17 | 31.13 | 26.58
 | 23.08 | 20.35 | 18.20 | 16.48
 | 15.12 | 14.04 | 13.20
 | 12.59 | 12.21 | 12.07
 | .5 |
| .7 | 139.0 | 126.9 | 101.8
 | 78.61 | 61.18 | 48.69
 | 39.70 | 33.11 | 28.16
 | 23.73 | 20.90 | 18.67 | 17.31
 | 15.48 | 14.37 | 13.50
 | 12.88 | 12.48 | 12.34
 | .6 |
| .9 | 157.4 | 142.4 | 112.4
 | 85.58 | 65.94 | 52.10
 | 42.26 | 35.10 | 29.76
 | 25.04 | 22.56 | 20.09 | 17.72
 | 16.59 | 15.36 | 14.12
 | 13.72 | 13.29 | 12.87
 | .9 |
 | | |
 | | |
 | | | |
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 | |
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 | | |
 | | | |
 | | |
 | | |
 | |
| 5.0 | 167.1 | 150.5 | 117.9
 | 89.15 | 68.36 | 53.83
 | 43.55 | 36.10 | . 30.56
 | 26.36 | 23.11 | 20.57 | 18.55
 | 16.95 | 15.69 | 14.72
 | 14.01 | 13.56 | 13.40
 | μR
5.0 |
| 5.0
.1
.2
.3 | 167.1
177.3
187.9
198.8 | 150.5
159.0
167.7
176.7 | 117.9
123.5
129.2
135.0
 | 89.15
92.76
96.42
100.1 | 68.36
70.80
73.26
75.74 | 53.83
55.57
57.31
59.07
 | 43.55
44.85
46.15
47.46 | 36.10
37.11
38.12
39.13 | . 30.56
31.37
32.17
32.98
 | 26.36
27.02
27.68 | 23.11
23.67
24.22 | 20.57
21.04
21.52 | 18.55
18.97
19.38
 | 16.95
17.32
17.69 | 15.69
16.02
16.36 | 14.72
15.02
15.33
 | 14.01
14.29
14.58 | 13.56
13.83
14.10 | 13.40
13.67
13.93
 | μR
5.0
.1
.2 |
| 5.0
.1
.2
.3
.4 | 167.1
177.3
187.9
198.8
210.3 | 150.5
159.0
167.7
176.7
186.0 | 117.9
123.5
129.2
135.0
141.0
 | 89.15
92.76
96.42
100.1
103.9 | 68.36
70.80
73.26
75.74
78.24 | 53.83
55.57
57.31
59.07
60.84
 | 43.55
44.85
46.15
47.46
48.77 | 36.10
37.11
38.12
39.13
40.14 | 30.56
31.37
32.17
32.98
33.80
 | 26.36
27.02
27.68
28.35
29.01 | 23.11
23.67
24.22
24.78
25.34 | 20.57
21.04
21.52
22.00
22.47 | 18.55
18.97
19.38
19.80
20.22
 | 16.95
17.32
17.69
18.06
18.43 | 15.69
16.02
16.36
16.69
17.02 | 14.72
15.02
15.33
15.63
15.94
 | 14.01
14.29
14.58
14.86
15.14 | 13.56
13.83
14.10
14.37
14.64 | 13.40
13.67
13.93
14.20
14.46
 | μR
5.0
.1
.2
.3
.4 |
| 5.0
.1
.2
.3
.4
.5
.6
.7 | 167.1
177.3
187.9
198.8
210.3
222.1
234.4
247.1 | 150.5
159.0
167.7
176.7
186.0
195.5
205.4
215.5 | 117.9
123.5
129.2
135.0
141.0
147.0
153.2
159.5
 | 89.15
92.76
96.42
100.1
103.9
107.7
111.5
115.4 | 68.36
70.80
73.26
75.74
78.24
80.76
83.30
85.85 | 53.83
55.57
57.31
59.07
60.84
62.62
64.41
66.20
 | 43.55
44.85
46.15
47.46
48.77
50.09
51.42
52.75 | 36.10
37.11
38.12
39.13
40.14
41.16
42.19
43.21 | . 30, 56
31, 37
32, 17
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Tabelle 2 (Fort.)

Rب	0 =0 ⁰	5°	10°	15 ⁰	20 ⁰	25°	30°	35°	40 ⁰	
10.0	1 333	910.1	504 6	308 2	206.9	14.8.9	112 8	88 97	72.38	
5	1 544	1 021	551.7	332 9	221.9	158 9	120.0	94 42	76.66	
11.0	1 775	1 138	599.9	357.8	237.0	169.0	127.3	99.89	80.95	
. 5	2 028	1 2 5 9	648.9	383.1	252.2	179.1	134.6	105.4	85.25	
			(00.0							
12.0	2 304	1 386	698.9	408.6	267.5	189.3	141.8	110.9	89.55	
	2 604	1 51/	749.6	434.3	282.9	199.5	149.1	116.4	93.86	
13.0	2 929	1 70/	962.2	460.2	290.5	209.0	120.2	127.9	102 5	
.,	5 280	1 / 74	0 / 3 . 2	400.3	313.0	220.0	105.0	127.4	102.5	
14.0	3 659	1 938	905.9	512.6	329.4	230.3	171.2	132.9	106.8	
. 5	4 065	2 086	959.3	539.0	345.1	240.7	178.5	138.4	111.2	
15.0	4 500	2 2 3 8	1 013	565.6	360.8	251.0	185.9	144.0	115.5	
. 5	4 965	2 393	1 067	592.3	376.5	261.4	193.3	149.5	119.8	
16.0	5 461	2 552	1 122	619.1	392.3	271.8	200.7	155.1	124.2	
. 5	5 989	2 714	1 177	646.0	408.2	282.2	208.1	160.6	128.5	
17.0	6 551	2 879	1 233	673.1	424.0	292.6	215.5	166.2	132.8	
. 5	7 146	3 046	1 289	700.2	439.9	303.1	222.9	171.6	:37.2	
19.0	7 776	3 2 16	1 3.5	727 /	455 0	313 5	2 30 /	177 3	141 5	
10.0	8 442	3 369	1 402	754 7	471 8	324.0	237.8	182.9	145.9	
19 0	9 145	3 564	1 4 5 9	782 1	457.8	334.4	245.3	188.5	150.2	
.5	9 986	3 741	1 516	809.5	503.5	344.9	252.7	194.1	154.6	
	/ 500	5 / 4 /	. ,							
20.0	10 670	3 921	1 573	837.0	519.5	355.4	260.2	199.7	159.0	
	11 490	4 103	1 631	864.6	535.9	365.9	267.6	205.2	163.3	
21.0	12 350	4 286	1 659	892.2	552.0	3/6.4	2/5.1	210.8	10/./	
• • •	13 250	4 4/2	1 /4/	919.8	200.1	300.9	202.5	210.4	172.0	
22.0	14 200	4 6 5 9	1 805	947.6	584.2	397.5	290.0	222.0	176.4	
. 5	15 190	4 848	1 864	975.3	600.3	408.0	297.5	227.6	180.5	
23.0	16 220	5 038	1 922	1 003	616.4	418.5	305.0	233.2	185.1	
.5	17 300	5 2 3 0	1 981	1 031	632.6	429.1	312.5	238.8	189.5	
24.0	18 430	5 423	2 040	1 059	648.7	439.6	319.9	244.4	193.9	
. 5	19 610	5 619	2 099	1 087	664.9	450.2	327.4	250.0	198.2	
25.0	20 830	5 8 1 4	2 158	1 115	631.1	460.7	334.9	255.6	202.6	
.5	22 110	6 012	2 217	1 143	697.3	471.3	342.4	261.2	207.0	
26 0	22 / 20	6 210	2 2 7 7		713 5	481 8	340.9	266 8	211 3	
20.0	26 810	6 4 10	2 336	1 199	729 7	407.4	357 4	272.4	215.7	
27 0	26 240	6 610	2 396	1 227	745.9	502.9	364.9	278.0	220.1	
17.0	27 730	6 812	2 4 56	1 255	762.1	513.5	372.4	293.6	224.4	
								200.2	220.0	
28.0	29 270	7 015	2 515	1 283	778.4	524.1	3/9.9	269.2	220.0	
	30 870	/ 218	2 5/5	1 311	794.0	534.7	30/.4	294.0	233.2	
29.0	32 520	7 423	2 635	1 3 3 9	010.9	343.2 EEC 0	394.9	306.1	241 9	
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30.0	36 000	7 834	2 755	1 395	843.4	566.4	409.9	311.7	246.3	
. 5	37 830	8 041	2 815	1 423	859.6	\$77.0	417.4	317.3	250.7	
31.0	39 720	8 249	2 875	1 4 5 2	875.9	587.6	424.9	322.9	255.0	
• 2	41 670	8 4 5 7	2 936	1 480	892.2	598.1	432.5	328.5	209.4	

450	500	550	600	650	700	750	800	85 ⁰	90 ⁰	Rىر
60.44	51.57	44.85	39.66	35.63	32.48	30.07	28.29	27.13	26.70	10.0
63.91	54.46	47.30	41.79	37.51	34.17	31.61	29.72	28.49	28.03	.5
67.38	57.35	49.76	43.92	39.39	35.86	33.16	31.16	29.85	29.36	11.0
70.86	60.24	52.22	46.06	41.27	37.55	34.70	32.59	31.22	30.70	.5
74.34	63.14	54.68	48.19	43.16	39.25	36.24	34.03	32.58	32.03	12.0
77.83	66.04	57.14	50.33	45.04	40.94	37.79	35.46	33.94	33.36	5
81.32	68.94	59.61	52.47	46.93	42.63	39.34	36.90	35.30	34.69	13.0
84.82	71.84	62.08	54.60	48.82	44.33	40.88	38.34	36.67	36.02	.5
88.31	74.74	64.54	56.74	50.70	46.02	42.43	39.77	38.03	37.36	14.0
91.81	77.65	67.01	58.88	52.59	47.72	43.97	41.21	39.39	38.69	.5
95.32	80.56	69.48	61.02	54.48	49.41	45.52	42.65	40.75	40.02	15.0
98.82	83.47	71.95	63.17	56.37	51.11	47.07	44.09	42.12	41.35	.5
102.3	86.38	74.43	65.31	58.26	52.80	48.62	45.52	43.48	42.69	16.0
105.8	89.29	76.90	67.45	60.15	54.50	50.16	46.96	44.84	44.02	.5
109.3	92.20	79.37	69.59	62.04	56.19	51.71	48.40	46.21	45.35	17.0
112.9	95.*2	81.84	71.73	63.93	57.89	53.26	49.84	47.57	46.69	.5
116.4	98.03	84.32	73.88	65.82	59.59	54.81	51.27	48.93	48.02	18.0
119.9	100.9	86.79	76.02	67.71	61.28	56.36	52.71	50.30	49.35	.5
123.4	103.9	89.27	78.17	69.60	62.98	57.90	54.15	51.66	50.68	19.0
126.9	106.8	91.74	80.31	71.49	64.68	59.45	55.59	53.02	52.02	.5
130.4	109.7	94.22	82.46	73.38	66.37	61.00	57.03	54.39	53.35	20.0
133.9	112.6	96.70	84.60	75.28	68.07	62.55	58.47	55.75	54.68	.5
137.5	115.5	99.17	86.75	77.17	69.77	64.10	59.90	57.12	56.02	21.0
141.0	118.4	101.6	88.89	79.06	71.46	65.65	61.34	58.48	57.35	.5
144.5	121.4	104.1	91.04	80.95	73.16	67.20	62.78	59.84	58,68	22.0
148.0	124.3	106.6	93.18	82.84	74.86	68.75	64.22	61.21	60.01	.5
151.5	127.2	109.1	95.33	84.74	76.56	70.29	65.66	62.57	61.35	23.0
155.1	130.1	111.6	97.47	86.63	78.25	71.84	67.10	63.94	62.69	.5
158.6	133.0	114.0	99.62	88.52	79.95	73.39	68.54	65.30	64.01	24.0
162.1	136.0	116.5	101.8	90.41	81.65	74.94	69.97	66.66	65.35	.5
165.6	138.9	119.0	103.9	92.31	83.35	76.49	71.41	68.03	66.68	25.0
169.2	141.8	121.5	106.1	94.20	85.04	78.04	72.85	69.39	68.01	.5
172.7	144.7	123.9	108.2	96.09	86.74	79.59	74.29	70.75	69.35	26.0
176.2	147.7	126.4	110.4	97.98	88.44	81.14	75.73	72.12	70.68	.5
179.7	150.6	128.9	112.5	99.57	90.14	82.69	77.17	73.48	72.01	27.0
183.2	153.5	131.4	114.6	101.8	91.84	84.24	78.61	74.85	73.35	.5
186.8	156.4	133.9	116.8	103.7	93.53	85.78	80.04	76.21	74.68	28.0
190.3	159.3	136.3	118.9	105.6	95.23	87.33	81.48	77.57	76.01	.5
193.8	162.3	138.8	121.1	107.4	96.93	88.88	82.92	78.94	77.34	29.0
197.3	165.2	141.3	123.2	109.3	98.63	90.43	84.36	80.30	78.68	.5
200.9	168.1	143.8	125.4	111.2	100.3	91.98	85.80	81.66	80.01	30.0
204.4	171.0	146.3	127.5	113.1	102.0	93.53	87.24	83.03	81.34	.5
207.9	174.0	148.7	129.7	115.0	103.7	95.08	88.67	84.39	82.68	31.0
211.4	176.9	151.2	131.8	116.9	105.4	96.63	90.11	85.75	84.01	.5



Fig.2. Konvergenzverlauf der numerischen Integration nach Gl.(4) für $\theta = 0^{\circ}$ und 90°. (a) und (b) Betrag des Integrationsfehlers $|\Delta I|$ in Abhängigkeit von der Intervallteilung $1/d\alpha$. Die schwach punktierten Kurvenstücke treten jeweils bei einem Vorzeichenwechsel von ΔI auf; massgebend für die Konvergenz sind die kräftig durchgezeichneten Enveloppen der Kurven. (c) Einfluss von A_{Zy1} -Ungenauigkeiten auf die Integrale A_{Kug} nach Gl.(4); $\theta = 90^{\circ}$, Teilung $1/d\alpha = 360/\pi$.

Tafel 5.3.6A der *International Tables* ersichtlich ein Übertragungsfehler eingeschlichen, der leider auch Folgefehler in der Tabelle 5.3.6B verursacht hat. Die übrigen Abweichungen, welche die Tabelle 1 erkennen lässt, sind dagegen gering; ihre Ursache darf wohl in erster Linie restlichen numerischen Ungenauigkeiten der Tabellen 5.3.6A zugeschrieben werden.

Ein Beispiel für eine erweiterte Anwendung der A_{Kug} -Tabelle

Es sei bemerkt, dass man mit der Schreibweise (4) des Absorptionsfaktorintegrals implizit auch einen wichtigen speziellen elliptischen Fall erfasst, nämlich den Fall des Rotationsellipsoids dessen Rotationssymmetrieachse c die Drehachse ist und das \perp c durchstrahlt wird (sogen. Äquatoraufnahme). Führt man vor der Substitution (3) eine lineare Dehnung in z-Richtung durch

$$z \rightarrow z' = (c/a)z$$

so wird die Kugel in ein Rotationsellipsoid mit den Achsen a=R und c=(c/a)R überführt; a wie r bleiben von der Dehnung unberührt, da sie senkrecht zur Dehnungsrichtung liegen. Man findet:

$$A_{\rm Ell} = \int_{-1}^{+1} r^2 \pi A_{\rm Zy1}(\mu r) dz' / (4\pi a^2 c/3)$$
$$= \frac{3}{4} \int_{-1}^{+1} \left(\frac{r}{a}\right)^2 A_{\rm Zy1}(\mu r) \frac{(c/a)dz}{(c/a)a}$$

das unter Beachten der Substitutionen (3) und nach Kürzen von Zähler und Nenner unmittelbar in (4) übergeht:

$$A_{\rm Ell} = A_{\rm Kug}(\mu a)$$
.

Diese Gleichung besagt, dass der Absorptionsfaktor $A_{\rm E11}$ des Rotationsellipsoides bei einer Durchstrahlung $\perp c$ unabhängig von der Länge der *c*-Achse ist und mit dem Wert $A_{\rm Kug}$ für R=a übereinstimmt (Weber, 1963).

Der Verfasser dankt der Deutschen Forschungsgemeinschaft auch an dieser Stelle vielmals für die finanzielle Unterstützung der vorliegenden Arbeit. Dank gebührt ferner dem Deutschen Rechenzentrum, mit dessen IBM-Anlage 7094 alle vorliegenden numerischen Berechnungen ausgeführt werden konnten.

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A System for the Coding and Generating of Layered, Tetrahedrally Close-Packed Structures

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A simple coding system is proposed which applies to those layered, tetrahedrally close-packed structures whose secondary nets may be generated by two sets of parallel (zigzag) lines (β -W, Friauf-Laves, μ , σ , P, M phases, *etc.*). This coding scheme represents a great condensation of structural data, from which atomic coordination can be regenerated; it enables one to recognize similarities between structures without plotting out all the atoms; and it indicates how new members of this structure family may be generated.

Introduction

Tetrahedrally close-packed structures (Frank & Kasper, 1958, 1959; Shoemaker & Shoemaker, 1967, 1969) contain interpenetrating triangulated coordination number (CN) 12, 14, 15, or 16 polyhedra which are in most cases generated by the alternate stacking of primary layers of pentagon-triangle, pentagon-hexagontriangle or hexagon-triangle nets of atoms with secondary layers of triangle, square-triangle or square nets of atoms, such that all pentagons of successive primary nets are covered antisymmetrically by pentagons of neighbouring primary nets, and similarly for the hexagons. The atoms of the secondary interleaving nets