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The Crystal Structure of Co_2Si*

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The crystal structure of Co_2Si has been redetermined from single-crystal X-ray data. The structure given by Borén, Ståhl & Westgren is incorrect. Co_2Si belongs to space group D_{2h}^{16}–*Pnam*, with 8 cobalt atoms and 4 silicon atoms in positions 4(*c*): $\pm(x, y, \frac{1}{4};\ \frac{1}{2}-x, \frac{1}{2}+y, -\frac{1}{4})$ with parameters Co_{I}: $x = 0{\cdot}038$, $y = 0{\cdot}218$; Co_{II}: $x = 0{\cdot}174$, $y = 0{\cdot}562$; Si: $x = 0{\cdot}702$, $y = 0{\cdot}611$. Co_2Si is isostructural with Rh_2Ge and has a distorted Ni_2In structure.

The programming of the calculation of the (001) Fourier projection on the I.B.M. No. 701 calculator is also described.

Introduction

A structure for Co_2Si was first proposed by Borén, Ståhl & Westgren (1935). Because it was apparently the first of a type, the *Strukturbericht* (1937) designated the Co_2Si structure, as proposed by the above authors, the *C*-37 type. Since its publication, apparently no other structure isomorphous with Co_2Si has been reported. Kripiakevich (1951) has shown that the structure reported by Borén *et al.* is a distorted Ni_2In structure.

One of us (S. G.) became interested in the Co_2Si structure while working on the rhodium–germanium system (Geller, 1955). The phase Rh_2Ge seemed to be isomorphous with Co_2Si. That is, there was a striking qualitative similarity between the powder photographs of the two compounds. Work with powder samples on

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the Norelco diffractometer confirmed the similarity. However, it began to appear from the latter work that the structure reported by Borén *et al.* was incorrect. Therefore, a single-crystal analysis was undertaken, which, as will be shown, proves conclusively that the structure given by Borén *et al.* is incorrect. It will also be shown that Co_2Si, Ni_2Si, Rh_2Ge and Rh_2B are isomorphous.

The Co_2Si was prepared by induction heating a proper mixture of cobalt and silicon, each of high purity, in an alundum crucible. A helium atmosphere was used.

A powder photograph with Fe $K\alpha$ radiation of some of the crushed product checked with the data reported by Borén *et al.* Confirmation of spacings was obtained by means of the Norelco diffractometer.

Determination of the structure

The crushed Co_2Si was examined carefully with a binocular microscope. A small crystal with cross section 0·1 × 0·1 mm. was isolated and mounted on a goniometer head. The crystal was aligned by application of the Hendershot (1937) method. Weissenberg photographs were taken, using Zr filtered Mo $K\alpha$ radiation. Three films interleaved with 0·001 in. Cu foil were used for each exposure (Hughes, 1941). The longest exposure given the zero layer was 72 hr.

The diffraction symmetry of the single-crystal photographs is D_{2h}–*mmm*. Reflections of the types $(h0l)$, h odd, and $(0kl)$, $k+l$ odd are absent. Thus the probable space groups are either D_{2h}^{16}–*Pnam* or C_{2v}^{9}–*Pna*. The cell constants by rough measurement were so nearly those given by Borén *et al.*, that it was decided to use them. However, because of the desire to adhere to convention, the a and b axes have been interchanged. Also, the values of Borén *et al.* have been multiplied by the factor 1·00202 to convert from what are undoubtedly kX. units to Å units. Thus the lattice constants are

$$a = 4\cdot918,\ b = 7\cdot109,\ c = 3\cdot738\ \text{Å}\ (\text{all}\ \pm 0\cdot003\ \text{Å})\,.$$

The crystal photographed had the c axis as rotation axis. The Weissenberg layer photographs about this axis looked very similar to corresponding photographs of an Rh_2Ge crystal (Geller, 1955). From this comparison it was quite obvious that the two compounds are isomorphous (space group D_{2h}^{16}–*Pnam**).

The relative intensities of the $(hk0)$ reflections were estimated visually by comparison with an intensity scale. The phases of the structure factors of the Rh_2Ge structure were applied to the observed F_{hk0} of the Co_2Si structure. This was justifiable because in the Rh_2Ge structure almost all of the phases of observable reflection amplitudes were determined by the rhodium atoms. In Co_2Si the cobalt atoms are obviously weighted even more heavily with respect to the silicon atoms than the rhodium atoms with respect to the germanium atoms in Rh_2Ge.

An electron density projection on (001) was computed on the I.B.M. No. 701 machine. Details of the computation are given in the Appendix. The parameters obtained from this projection were used to calculate reflection amplitudes. There were only seven changes of sign out of 100 reflections strong enough to be observed. A correction grid was calculated using Beevers–Lipson strips (Beevers & Lipson, 1936; Beevers, 1952). The corrections were applied to the original projection. Only two of the six parameters changed, and these by 0·001. The final parameters are shown in Table 1.

Table 1. *Atomic coordinates in* Co_2Si

	Atomic coordinates		
Atom	x	y	z
Co_I	0·038	0·218	$\frac{1}{4}$
Co_{II}	0·174	0·562	$\frac{1}{4}$
Si	0·702	0·611	$\frac{1}{4}$

No series-termination correction was made. It is felt that such correction, if any, would be extremely small. since reflections from far out in the reciprocal lattice have been used. Satisfactory convergence was indicated by absence of sizable spurious peaks.

The comparison of observed and calculated $(hk0)$ amplitudes is shown in Table 2. Values of atomic scattering factors are averages of those taken from the *International Tables* (1935) and from Pauling & Sherman (1932). A temperature factor

$$[-0\cdot68\times10^{-16}\,(\sin\theta/\lambda)^2]$$

was applied to the calculated structure factor values. No correction was made for absorption. The value of the discrepancy factor, R, for the $(hk0)$ reflection amplitudes is 0·13, excluding those for which intensities were too weak to be observed.

Discussion of the structure

The relation of the Ni_2In structure (Laves & Wallbaum, 1942) to the NiAs structure (Aminoff, 1923)

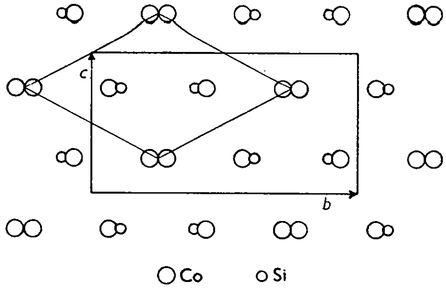

Fig. 1. The (100) projection of Co_2Si, indicating relation to Ni_2In-type structure.

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* In these compounds the layer photographs with l odd are similar, as are those with l even, indicating *Pnam* to be the most probable space group.

Table 2. *Comparison of calculated with observed reflection amplitudes*

		Amplitude	
	(k)	Obs.	Calc.
h=0	2	10	-11
	4	14	17
	6	65	-63
	8	23	-18
	10	<8	2
	12	17	-18
	14	21	18
	16	<9	0
	18	14	15
h=1	1	13	-12
	2	29	-23
	3	61	-59
	4	38	-34
	5	47	45
	6	56	-59
	7	16	-20
	8	<7	4
	9	42	44
	10	12	16
	11	9	-12
	12	29	26
	13	<10	4
	14	<10	7
	15	<10	-7
	16	<9	-3
	17	<8	-6
	18	<7	-6
	19	<6	3
h=2	0	5	-5
	1	<4	2
	2	124	-93
	3	106	89
	4	61	57
	5	17	21
	6	11	13
	7	<7	4
	8	9	7
	9	10	-6
	10	8	11
	11	18	-16
	12	9	-9
	13	<10	4
	14	9	10
	15	10	-11
	16	18	-15
	17	<8	6
	18	<7	1
	19	<6	3
h=3	1	55	47
	2	24	-28
	3	6	8
	4	20	22
	5	24	29
	6	8	-9
	7	68	-56
	8	25	25
	9	14	-14
	10	18	-19
	11	24	-21
	12	<9	2
	13	19	15
	14	<10	-3
	15	16	11
	16	<9	2
	17	<8	5
	18	<7	3
	19	<5	4
h=4	0	21	20
	1	72	-71
	2	30	-35
	3	23	-27
	4	8	9
	5	41	-41
	6	<7	-2
	7	8	7
	8	9	12
	9	12	12
	10	9	13
	11	<9	0
	12	<10	-8
	13	20	20
	14	<9	2
h=4	15	<9	-2
	16	10	-9
	17	<8	5
	18	<6	2
h=5	1	9	-3
	2	7	7
	3	20	-25
	4	47	47
	5	<8	2
	6	9	-10
	7	8	8
	8	21	21
	9	30	28
	10	26	24
	11	<10	1
	12	<10	-2
	13	<9	-5
	14	9	-9
	15	<9	-8
	16	<8	-1
	17	<7	-4
	18	<5	5
h=6	0	36	38
	1	18	-17
	2	13	17
	3	49	42
	4	<8	0
	5	9	-11
	6	17	-18
	7	<9	-4
	8	18	-18
	9	<9	2
	10	<10	-9
	11	<10	-6
	12	<10	-2
	13	<10	9
	14	<9	7
	15	12	-11
	16	<7	6
	17	<6	5
h=7	1	9	-14
	2	24	-20
	3	<9	4
	4	<8	-4
	5	<9	8
	6	43	-36
	7	<9	5
	8	16	14
	9	<10	-3
	10	<10	-2
	11	<10	1
	12	25	20
	13	<9	1
	14	<8	3
	15	<8	0
	16	<6	-1
h=8	0	29	-28
	1	20	-17
	2	<9	-6
	3	24	22
	4	<9	1
	5	<9	3
	6	9	13
	7	14	10
	8	11	8
	9	<10	0
	10	<10	2
	11	18	-15
	12	<9	4
	13	<8	1
	14	<7	-4
	15	<7	-7
	16	<4	-2
h=9	1	14	14
	2	<10	-7
	3	11	9
	4	11	13
	5	15	-14
	6	<10	-3
	7	<10	-4
	8	11	13
	9	18	14
	10	16	-12
	11	<8	1
	12	<8	-1
	13	<7	-1
	14	<6	-3
h=10	0	9	-6
	1	14	-14
	2	9	9
h=10	3	<10	-4
	4	10	-10
	5	12	-15
	6	<9	2
	7	<9	-4
	8	<9	4
	9	<9	5
	10	<8	0
	11	<7	4
	12	<6	3
	13	7	9
h=11	1	10	-10
	2	<9	6
	3	<9	1
	4	12	10
	5	<9	-5
	6	<9	-3
	7	15	14
	8	<8	2
	9	<8	0
	10	<7	-4
	11	6	6
h=12	0	<8	-3
	1	<8	0
	2	15	12
	3	<8	6
	4	<8	-3
	5	<8	2
	6	<7	-1
	7	<7	1
	8	<6	6
	9	<5	-1
h=13	1	<6	-2
	2	<6	-6
	3	<6	5
	4	<7	-6
	5	<5	-4

has been described in the paper on the rhodium–germanium system (Geller, 1955). In the latter paper, it was shown also that Rh_2Ge, Rh_2B (Mooney & Welch, 1954) and δ-Ni_2Si (Toman, 1952) are isostructural and have a distorted Ni_2In structure. As has been stated above, Co_2Si is also isostructural with these.

Table 3. *Interatomic distances in* Co_2Si

(Values in Å units.)

Co_I:	8 Co	2 Co_I	at 2·50(2)
		6 Co_{II}	at 2·52, 2·59(2), 2·65(2), 2·68
	6 Si		at 2·34(2), 2·47, 2·57(2), 3·25
Co_{II}:	8 Co	2 Co_{II}	at 2·68(2)
		6 Co_I	at 2·52, 2·59(2), 2·65(2), 2·68
	5 Si		at 2·32(2), 2·33, 2·35, 2·62
Si:	11 Co	6 Co_I	at 2·34(2), 2·47, 2·57(2), 3·25
		5 Co_{II}	at 2·32(2), 2·33, 2·35, 2·52
	4 Si		at 3·15(2), 3·15(2)

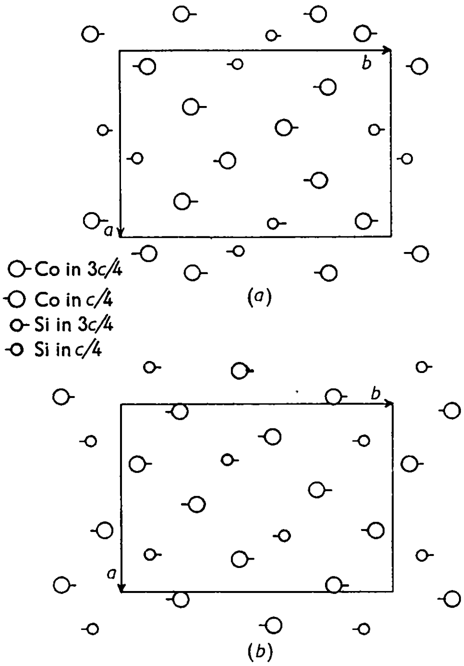

Fig. 2. (*a*) The (001) projection of the incorrect Co_2Si structure. (*b*) The (001) projection of the correct Co_2Si structure.

The interatomic distances in Co_2Si are listed in Table 3. Figs. 1 and 2(*b*) indicate the arrangement of atoms in the structure. There are eight Co atoms coordinated to the Co_I atom at distances 2·50–2·68 Å. Six of these eight atoms, the Co_{II} atoms, form a distorted octahedron. The two Co_I atoms coordinated to the Co_I atom lie one above and one below it. There are also five Si atoms coordinated to the Co_I atom at distances 2·34–2·57 Å. Including a Si atom at distance 3·25 Å, the Si atoms also lie at the corners of a distorted octahedron. The Co_{II} atoms have a somewhat different kind of coordination. The Co_{II} atom is coordinated to eight Co atoms at distances 2·52 to 2·68 Å. The six Co_I atoms form a distorted trigonal prism. The five Si atoms at distances 2·32–2·62 Å are at the corners of a trigonal bipyramid. Each Si atom is coordinated to six Co_I atoms (five at distances 2·34–2·57 Å and the sixth at 3·25 Å) at the corners of a distorted trigonal prism and to five Co_{II} atoms at the corners of a trigonal bipyramid. It should be noted (see Table 3) that the Si–Si distances are all long and cannot really be said to be contacts.

As in the cases of the Rh_2Ge, direct application of Pauling's (1949) resonating-valence-bond theory to the Co_2Si structure leads to unsatisfactory results. If the valences of the atoms are computed by assigning bond numbers to each of the bonds by use of the relation

$$D_n = D_1 - 0{\cdot}600 \log n ,$$

in which D_n is the observed interatomic distance, D_1 is the sum of the single bond radii (as in Pauling's paper), and n is the bond number, one obtains for the valence of Co_I, 6·7; of Co_{II}, 6·9; and of Si 7·7. The value obtained for the silicon valence is much too high and is indicative of the complexity of the bonding in this compound.

Thus far it is believed that only four intermetallic compounds with the distorted Ni_2In structure and isostructural with Co_2Si have been found. These are Rh_2Ge, Rh_2B, δ-Ni_2Si and Co_2Si. The average interatomic distances in these compounds are listed in Table 4. It should be noted that in all cases the average metal–metal distance is 4–5·6% larger than the elemental diameter of the metal, whereas, in the case of the metal–metalloid distance, the average is equal to the sum of the elemental radii. In the case of boron, it is really not justifiable to assign to it the radius obtained from the elementary boron structure (Hughes & Hoard, 1954; see also Hoard, Geller & Hughes, 1951) since in the latter the bonding would be expected to be highly covalent. The metalloid–metalloid distances are all very large (see Geller, 1955) and cannot be called real contacts.

Table 4. *Average interatomic distances in* Co_2Si *isomorphs*

Compound	*M–M* (Å)	*M–B* (Å)
Rh_2Ge	2·82 (2·68)	2·57 (2·56)
Rh_2B	2·82 (2·68)	2·56 (?)
δ-Ni_2Si	2·64 (2·50)	2·42 (2·42)
Co_2Si	2·60 (2·50)	2·42 (2·42)

Numbers in parenthesis are the elemental radii sums.

The (001) projection of the structure obtained by Borén *et al.* is shown in Fig. 2 together with that found by the present authors.

The structure proposed by Borén *et al.* gives a short Si–Si distance of 2·15 Å. These authors point out that this is abnormal but that such distances are not unusual in silicides of iron or neighboring transition metals. The latter is not so because the Si–Si distance is about 2·76 Å in the FeSi-type (Phragmén, 1923; Wever & Moeller, 1930; Borén, 1933; Pauling & Soldate, 1948) structures, including FeSi, NiSi and CoSi, to which Borén refers. This is considerably longer than the elemental diameter of 2·34 Å, though not as long as the Si–Si distances of 3·27 Å in δ-Ni_2Si, 3·29 Å in θ-Ni_2Si and 3·15 Å in Co_2Si.

It is noteworthy that in CoSi the average Co–Co distance is 2·73 Å as against 2·60 Å in Co_2Si. Thus, whereas the average Si–Si distance in Co_2Si is longer than in CoSi, the average Co–Co distance is shorter in Co_2Si than in CoSi. But the average Co–Si distance in the two compounds does not change much (if at all) from the sum of the elemental radii. The average Co–Si distance in CoSi is 2·38 Å.

APPENDIX

Projection Fourier calculations on the I.B.M. 701 calculator

The Fourier calculation of projections is a task very well suited for automatic digital computing equipment because of the relatively simple but highly repetitive nature of the computations and because numerous cases, sufficiently similar to be readily handled by the same general machine program, are likely to occur over a period of time. The following formulation was chosen as a basis for planning machine programs since it was considered sufficiently general to meet our needs in the foreseeable future without being so general as to be inefficient for the cases actually at hand:

Given the positive integers H, K, M, N and the real numbers A, B, C, D, p, q and $a_{hk}, b_{hk}, c_{hk}, d_{hk}$, $(h = 0, 1, \ldots, H;\ k = 0, 1, \ldots, K)$, calculate

$$\begin{aligned} S(x, y) = {} & A \sum_{k=0}^{K} \sum_{h=0}^{H} a_{hk} \cos hx \cos ky \\ & + B \sum_{k=0}^{K} \sum_{h=0}^{H} b_{hk} \sin hx \sin ky \\ & + C \sum_{k=0}^{K} \sum_{h=0}^{H} c_{hk} \cos hx \sin ky \\ & + D \sum_{k=0}^{K} \sum_{h=0}^{H} d_{hk} \sin hx \cos ky \end{aligned}$$

for $x = 0, p, 2p, \ldots, Np$; $y = 0, q, 2q, \ldots, Mq$.

A program for performing this calculation was written for the I.B.M. Electronic Data Processing Machines Type 701 and Associated Equipment, briefly known as the '701', and was tested and used on the 701 at the World Headquarters of the International Business Machines Corporation in New York City. The high-speed random-access storage of this machine consists of cathode ray tubes capable of holding 4096 numbers consisting of 35 binary digits and sign—so called full words, roughly equivalent to 10-digit decimal numbers —or 8192 numbers or instructions consisting of 17 binary digits and sign, called half words. Practically unlimited auxiliary storage is available on magnetic drums and tapes. Restricting the parameters of the problem by the inequalities $H \leq 27$, $K \leq 30$, $M \leq 30$, $N \leq 45$, top speed and simplicity of programming were achieved by operating entirely within the high-speed memory, by accumulating all final results in memory for a single print-out operation at the end of the problem, by using full words throughout to simplify scaling of intermediate results, etc., but it should be emphasized that it was by no means necessary to impose any such restrictions.

The time required to add two full or half words in the 701, one placed in the arithmetic unit and the other located anywhere in high speed storage, is 60 microsec., and to multiply them, 456 microsec. or less, depending on the operations that follow. Most logical operations, such as deciding between two courses of action depending on the value or sign of the quantity standing in the accumulator, take place in 48 microsec. Even at these speeds, the calculating time for any problem of appreciable size becomes substantial enough—compared to the times for reading in data and instructions and printing results (largely determined by the mechanical speeds of a conventional card reader and printer)—to make the choice of a time-saving method of calculation desirable. To this end, the double summations in the present problem were naturally performed by first forming and storing the single sums with respect to one summation index (e.g. $\sum_{k=0}^{K} a_{hk} \cos ky$) for all values of the other index, h, and one fixed value of the variable, y, then computing $S(x, y)$ for all values of the other variable, x, before repeating the process for the next value of y. Also, provisions were made by a simple test to bypass the calculation of any sums in the expression for $S(x, y)$ with the corresponding factor, A, B, C or D equal to zero. However, the most significant problem from a time standpoint appears to be the choice of a method for obtaining the values of the trigonometric functions involved. The standard procedure of calculating each sine or cosine from its power series (by a so-called sub-routine) each time it is needed would be prohibitively slow in this application. An attractive method, which should be explored further, is that of storing a table of all values of trigonometric functions needed in the problem (at most $M+N$ numbers, if $Np = Mq = 180°$). The method chosen because of its simplicity, flexibility and relatively high speed was that of obtaining each sine and cosine from those of the next lower value of the argument by the well known formulas for the cosine and sine of the sum of two arguments. With this method, the total calculating time for the case $H = 13$, $K = 21$, $N = M = 30$, $C = D = 0$, was approximately 2 min. To this should be added about 3 min. for card reading, printing, etc. The time required for a relatively inexperienced programmer to prepare and test the program was about 10 days, including about 1 hr. of machine time. The program (in which no emphasis was placed on minimization) consists of about 400 instructions, not counting the already existing sub-routines for loading and converting input data and instructions and converting and printing results.

No checks for possible machine errors were incorporated into the program (excluding the above mentioned sub-routines) since the short operating time would make re-runs of suspicious-looking cases readily feasible and since it was felt that the effects of a machine error most probably would be easily recognizable in analyzing the results.

The authors wish to acknowledge the aid given by Mrs J. Gaskill, who carried out the computations of the structure factors.

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