PRECISION MEASUREMENTS OF THE LATTICE CONSTANTS OF TWELVE COMMON METALS

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ABSTRACT

The lattice constant a has been determined within 0.1 percent (.03 percent for W) for *aluminum, iron, nickel, copper, molybdenum, palladium, silver, tungsten, platinum, gold, lead and bismuth,* by direct comparison with NaCl, $a(\text{NaCl}) = 2.814$ A. As pure samples as could be obtained were used, from 99.55 percent for Ni to 99.9995 percent for tungsten, and in many cases commercially pure samples were also measured for comparison. The results for the purest samples are summarized in Table XIII. The *density from the x-ray* data is in each case (except Al and Ag) greater than the density of the bulk metal as given in the literature, the difference being rather large for Mo (10.21 vs 9.1), for Pd (12.25 vs 11.9) and W (19.32 vs 18.77). For pure W remarkably sharp lines were obtained. For Bi a piece of a single artificial crystal was used.

PRECISION measurements of the lattice constants of metals have the same fundamental relation to metallurgical work that measurements of wave-lengths have to light. It is the purpose of this article to record the results of such measurements of the lattice parameter, distance of closest approach of atomic centers, and density, for some of the common metals. Some of the specimens were extremely pure. Samples of commercial purity were also obtained for most of these same metals so that an idea might be gained as to the distortion in the lattice to be expected from small amounts of the usual commercial impurities. The original sources of the samples and the purity claimed for each are given in connection with the various tables of x-ray data.

In every case the metal was diluted with cornstarch according to an empirical schedule[1] to reduce its opacity to a value approaching that of NaCl, and was then packed into one end of a capillary specimen tube of Corning 707BM glass. NaCl was packed into the other end of the tube as a calibration standard.[2] As has been pointed out by Havighurst, Mack and Blake[3] there are some real advantages in mixing the NaCl directly with the specimen to be examined. There is this disadvantage, however, that when the lines from the metal fall very near the lines from the NaCl, a good reading cannot be made on either. For this reason, even when

[1] Davey, Gen. Elec. Rev. 1925
[2] Davey, Phys. Rev. **19,** 538 (1922)
[3] Havighurst, Mack and Blake, J. Amer. Chem. Soc. **46,** 2368 (1924)

there was no possibility of chemical action between the NaCl and the metal, the technique originally described[2] was adopted.

The apparatus was the standard equipment described elsewhere,[4] using the alpha lines of the Mo K series. Each interplanar spacing smaller than 2.00 was made to give a value of the side a of the unit-cube by means of the proper theoretical factor. All such values for each film were solved graphically[5] for the most probable value. The final value of a for the pure samples is the average of at least two such most probable values. The uncertainty of reading of each of the lines of any given diffraction pattern is considered to be $\pm .002$A from 2.00A to 1.00A, and $\pm .001$A below 1.00A. This gives a reproducibility of ± 0.1 percent in the most probable value of a for any one film. In the single case of the two pure samples of tungsten, the lines were so narrow and so sharply defined that the reproducibility was considered to be 0.03 percent. In all cases the intensities assigned to lines are merely relative. Thus 4 is stronger than 3, and weaker than 5, but it is not intended that 4 shall be considered to be twice as strong as 2, nor half 8. All measurements of distances are in terms of the lattice parameter of NaCl, 2.814A.

The data are presented in the following tables. The results for the purest samples are summarized in Table XIII. For comparison with densities calculated from x-ray data, the values obtained by ordinary measurement are given as recorded in Van Nostrand's Chemical Annual and in Groth's Chemische Krystallographie.

TABLE I

Aluminum (atomic number 13; atomic weight 27.1). Face-centered cubic pattern

Data from a specimen of 99.97 percent Al from J. D. Edwards, Asst. Director of Research, Aluminum Company of America.

Plane	Intensity	Spacing (1)	Spacing (2)
111	10	2 34	2.34
100	9	2.02	2.03
110	8	1.431	1.432
311	10	1.221	1.220
111 (2)	5	1.170	1.168
100 (2)	4	1.013	1 012
331	7	.928	.928
210	7	.905	.905
211	5	.825	.825
511; 111(3)	6	.778	.778
110 (2)	2	.715	.715
	Side of unit cube	4.047A	4.046A
	Average	4.046 $\pm$ .004A	

[4] Davey, J. Opt. Soc. Amer. **5,** 479 (1921)
Gen. Elec. Rev. **25,** 565 (1922)

[5] Whipple, J. Frank. Inst. **182,** 37-205 (1916)

TABLE II

Iron (atomic number 26; atomic weight 55.84). Body centered cubic pattern

Data in columns (1) and (2) are from Fe made by Dr. R. W. Moore of this laboratory by reduction of "c.p." Fe_2O_3 by hydrogen.

Data in columns (3) and (4) are from vacuum fused electrolytic Fe from the Bureau of Standards, having the composition: 0.020 percent C; 0.001 percent Mn; 0.004 percent P; 0.017 percent S; 0.021 percent Si; 99.937 percent Fe (by difference).

Plane	Intensity	Spacing (1)	(2)	(3)	(4)
110	10	2.03	2.02	2.02	2.02
100	5	1.435	1.429	1.426	1.428
211	8	1.169	1.167	1.165	1.166
110 (2)	5	1.010	1.011	1.010	1.010
310	6	.905	.905	.903	.903
111	2	.825	.826	.824	.829
321	6	.764	.764	.763	.763
100 (2)	1	.....	.714		
110(2); 411	3	.673			
210	2	.638			
332	2	.608			
211(2)	2	.582			
Side of unit cube		2.857A	2.859A	2.855A	2.856A
Average		2.858 ± .003A		2.855 ± .003A	

TABLE III

Nickel (atomic number 28; atomic weight 58.68). Face-centered cubic pattern

The data are from a specimen made by Dr. R. W. Moore of this laboratory by reduction by hydrogen of oxide from the J. T. Baker Chemical Company, which has the following analysis: 0.275 percent Fe; 0.170 percent Co; 0.000 percent Cu; 0.005 percent SO_3; 0.002 percent Cl; 99.548 percent Ni (by difference).

Plane	Intensity	Spacing (1)	(2)
111	8	2.01	2.02
100	7	1.741	1.743
110	6	1.233	1.235
311	7	1.053	1.055
111(2)	5	1.009	1.011
100(2)	4	.875	.876
331	5	.804	.804
210	5	.782	.783
211	5	.716	.717
Side of unit cube		3.496A	3.502A
Average		3.499 ± .005A	

TABLE IV

Copper (atomic number 29; atomic weight 63.57). Face-centered cubic pattern

Column (1) contains data from commercial "conductivity" copper such as is ordinarily used in the electrical industry. Such copper is usually considered to be 99.98 per cent Cu. The remainder is largely Cu_2O. The solubility of oxygen in copper is less than 0.009 percent.[6] It exists mostly as segregations of Cu_2O in the crystals and at the crystal boundaries. These segregations may be seen under the microscope in the form of a Cu_2O-Cu eutectic, presumably composed of unit crystals of Cu_2O dispersed in Cu. It is not surprising, therefore, that "conductivity" copper should show, within experimental error, the same lattice parameter as the purest copper. Column (2) contains data of some finely divided copper used in some catalysis work of Professor A. Benton. The data in column (3) are from copper from the J. T. Baker Chem. Co. The impurities are not more than .01 percent.

Plane	Intensity	Spacings (1)	(2)	(3)
111	7	2.08	2.08	2.08
100	6	1.798	1.799	1.797
110	5	1.271	1.271	1.270
311	6	1.083	1.084	1.084
111(2)	4	1.038	1.038	1.038
100(2)	2	.900	....	.899
331	4	.826	.826	.825
210	3	.806	.805	.804
211	3	735	.735	.734
	Side of unit cube	3.598A	3.598A	3.596A
	Average		3.597 ± .004A	

TABLE V

Molybdenum (atomic number 42; atomic weight 96.0). Body centered cubic pattern

Columns (1) and (2) are from some Mo powder furnished by W. L. Enfield and G. E. Inman, of the Lamp Development Laboratory, National Lamp Works of the General Electric Company. The crystals of the powder are 99.8 percent Mo. Columns (3) and (4) are from Mo powder having a purity of 98 percent furnished by Dr. R. W. Moore of this laboratory. It is a good grade of commercial Mo.

Plane	Intensity	Spacings (1)	(2)	(3)	(4)
110	10	2.23	2.22	2.22	2.21
100	8	1.573	1.572	1.569	1.565
211	10	1.283	1.281	1.282	1.279
110 (2)	7	1.112	1.110	1.111	1.107
310	9	.994	.992	.993	.991
111	4	.908	.907	.905	.905
321	8	.840	.839	.839	.838
100(2)	3	——	.785	.784	.784
411; 110 (3)	6	.742	.740	.739	.739
210	5	.703	.702	.701	.702
	Side of unit cube	3.144A	3.139A	3.138A	3.134A
	Average	(99.8%) 3.142 ± .003A;		(98%) 3.136A	

[6] Hanson, Marryat and Ford, Research Reports of the British Non-ferrous Metals Research Assn. **13***B*, 223, (April 1924).

TABLE VI

Palladium (atomic number 46; atomic weight 106.7) Face-centered cubic pattern

This sample was given me by Dr. W. E. Forsythe, Director of the Nela Research Laboratory, National Lamp Works of the General Electric Co. It came originally from Englehardt under the specification of "Heraeus Pd" and was part of the metal used by Dr. Forsythe in determining the melting point of Pd as a standard for temperature measurement.

Plane	Intensity	Spacings (1)	(2)
111	8	2.21	2.20
100	8	1.925	1.921
110	7	1.363	1.361
311	9	1.163	1.161
111(2)	3	1.114	1.113
100(2)	3	.965	.964
331	7	.885	.885
210	7	.863	.863
211	5	.788	.788
511; 111(3)	6	.743	.743
110(2)	2	.683	.683
531	5	.654	.653
110(3); 221	5	.645	.644
310	3	.612	
	Side of unit cube	3.860A	3.858A
	Average	3.859 ± .003A	

TABLE VII

Silver (atomic number 47; atomic weight 107.88). Face-centered cubic pattern

Data given in columns (1) and (2) are for a sample originally from Professor G. Baxter, of "atomic weight" purity, 99.999 percent. Data given in columns (3) and (4) are for "fine silver" from our laboratory stock, considered to be 99.9 percent Ag. The other 0.1 percent is Cu. The difference in lattice parameters of the two specimens is at least five times the uncertainty of measurement.

Plane	Intensity	Spacings (1)	(2)	(3)	(4)
110	10	2.37	2.36	2.35	2.35
100	8	2.05	2.04	2.03	2.03
110	8	1.442	1.443	1.436	1.435
311	9	1.230	1.233	1.225	1.225
111(2)	5	1.178	1.178	1.173	1.172
100(2)	2	1 019	1.020	1.013	1.014
331	6	.935	937	.930	.931
210	6	912	.912	.908	908
211	4	.833	.832	828	828
511; 111(3)	4	.785	.786	.781	780
110(2)	1	.721			
531	3		.689		
110(3); 221	3		.680		
310	2		.645		
533	1		.622		
	Side of unit cube	4 079A	4 080A	4 059A	4.058A
	Average	(99.999%)4.079 ± .004A;		(99.9%)4 058A	

TABLE VIII

Tungsten (atomic number 74; atomic weight 184.0). Body-centered cubic pattern

Data in columns (1) and (2) are for samples from W. L. Enfield and G. E. Inman, of the Lamp Development Laboratory of the National Lamp Works of the General Electric Company. That for column (1) was 99.9995 percent W if we disregard traces of "impurities" which apparently are held only mechanically by the crystals. That for column (2) was 99.997 percent W. The remaining 0.003 percent was Mo. The lines on these two films were especially narrow and sharp. The reproducibility of readings of these films was so much better than for our ordinary diffraction patterns, that it seems justifiable to claim a reproducibility of 0.03 percent in the final value of the side of the unit-cube. Data in column (3) are for a filament from a 40-watt Mazda lamp. Six strands of the filament were packed together in one end of a glass specimen tube so as to insure a nearly random orientation of crystals with respect to the axis of the wires. Even with this precaution, lines are missing from the 310 and 210 planes. The lines on the film were not as narrow as those for columns (1) and (2), and the reproducibility of results is not greater than the customary 0.1 percent. Data in columns (4) and (5) are for commercially pure (98.58 percent) W supplied by Dr. R. W. Moore of this laboratory. The discrepancies between columns (4) and (5) are real, and are not to be accounted for by errors in reading the films.

Plane	Intensity	Spacing (1)	(2)	(3)	(4)	(5)
110	8	2.23	2.24	2.22	2.24	2.24
100	5	1.579	1.580	1.580	1.578	1.583
211	6	1.289	1.289	1.288	1.288	1.292
110(2)	5	1.116	1.115	1.114	1.115	1.117
310	6	.997	.997	....	.998	1.000
111	3	.912	.911	.911	.911	.913
321	5	.842	.843	.843	.844	.845
100(2)	2	.788	.788	.790	.788	.790
411; 110(3)	4	.744	.744	.744	.744	.745
210	4	.706	.706	....	.706	.706
332	1			.673		
211(2)	1			.645		
Side of unit cube		3.155A	3.155A	3.157A	3.156A	3.161A
Average		(pure) 3.155 ± .001A		———	(99.58%) 3.158 ± .003A	

TABLE IX

Platinum (atomic number 78; atomic weight 195.2). Face-centered cubic pattern

Data in Columns (1) and (2) are from a sample 99.995 percent Pt from the Bureau of Standards. Data in column (3) are from commercial Pt which probably contains a little Ir.

Planes	Intensity	Spacing (1)	(2)	(3)
111	7	2.27	2.26	2.26
100	6	1.956	1.956	1.957
110	6	1.385	1.383	1.383
311	7	1.179	1.181	1.180
111(2)	4	1.130	1.130	1.130
100(2)	2	.978	.978	.979
331	5	.897	.898	.897
210	5	.875	.875	.875
211	4	.798	.799	.798
511; 111(3)	3	.753	.753	.753
Side of unit cube		3.912A	3.913A	3.913A
Average			3.912 ± .004A	

TABLE X

Gold (atomic number 79; atomic weight 197.2). Face-centered cubic pattern

Data in columns (1) and (2) are from a sample of 99.999 percent Au from the San Francisco mint. Data in columns (3), (4), and (5) are from ordinary 24 carat gold.

Planes	Intensity	Spacing (1)	(2)	(3)	(4)	(5)
111	8	2.35	2.35	2.35	2.35	2.35
100	6	2.03	2.03	2.04	2.04	2.04
110	6	1.436	1.437	1.437	1.439	1.441
311	7	1.225	1.226	1.227	1.229	1.229
111(2)	5	1.173	1.173	1.174	1.175	1.177
100(2)	3	1.016	....	1.018	1.018	1.019
331	6	.933	.933	.934	.934	.936
210	6	.909	.909	.911	.911	.911
211	4	.830	.830	.831	.831	.832
511; 111(3)	4		.783	.784	.784	.784
Side of unit cube		4.064A	4.066A	4.071A	4.072A	4.076A
Average		(pure) 4.065 ± .004A,		(24 carat) 4.073 ± .004A		

TABLE XI

Lead (atomic number 82; atomic weight 207.20). Face-centered cubic pattern

Data for commercially pure lead. No analysis was available for the sample actually used, but such lead is usually considered to be 99.96 percent Pb.

Planes	Intensity	Spacing (1)	(2)
111	6	2.81	2.82
100	5	2.44	2.44
110	5	1.732	1.737
311	6	1.480	1.479
111(2)	2	1.415	1.415
100(2)	4	1.230	1.230
331	4	1.128	1.128
210	3	1.099	1.100
211	3	1.005	1.005
511; 111(3)	2	.947	.949
110(2)	2	.871	.870
531	1	.833	.832
100(3); 221	1	.821	.821
310	1	....	.779
Side of unit cube		4.919A	4.921A
Average		4.920 ± .005A	

TABLE XII

Bismuth (atomic number 83; atomic weight 209.02). Rhombohedral pattern. Structure two interpenetrating face-centered rhombohedra.

The specimen was a portion of a single crystal of Bi grown from the molten metal by Dr. S. L. Hoyt of this laboratory. Although no analysis was made of the composition of this crystal, it is assumed from the method of its growth that it can be properly classed as "pure." The axial ratio $c = 2.606$ was taken from Groth. It agrees within experimental error with that indicated by the graphical solution for structure.[7]

Plane	Intensity	Spacing (1)	Spacing (2)
00.1(1)(3)	1	3.93	3.94
10.1	1	3.70	3.72
10.2	9	3.26	3.27
10.4	8	2.35	2.36
11.0	8	2.26	2.27
10.5	3	2.02	2.03
00.1(2)(6); 11.3	4	1.964	1.970
10.1(2)	7	1.862	1.864
10.2(2)	6	1.635	1.637
10.7	3	1.550	1.554
20.5	2	1.511	....
11.6	6	1.486	1.489
12.2	7	1.439	1.441
10.8	2	1.383	1.387
12.4	4	1.326	1.328
10.0(1)(3)	4	1.310	1.312
20.7	2	1.283	1.283
12.5	1	1.257	1.257
20.8	2	1.182	....
11.9	3	1.137	1.137
12.7	1	1.116	1.116
22.3; 30.6	3	1.091	1.093
31.2	3	1.072	1.073
12.8	2	1.046	1.047
31.4	2	1.021	1.023
00.12	2	.984	.986
40.2	2	.967	....
40.4	2	....	.931
32.2	2	.890	.892
31.8	1	.876	....
41.0; 22.9	1	.857	.858
32.7	2	.792	....
33.0	2	.750	....
	Side of unit triangle	4.536A	4.543A
	Average	4.539 ± .005A	

Note: For planes 20·1; 12·1; 00·9; 10·1(3); 22·0; 10·10; 31·1; 10·11; 20·10; 41·1; 31·5; 22·6; 20·11; 21·10; 30·9; 31·7; 40·5; 32·1; 10·13; 21·11; 32·4; 40·7; 32·5; 41·3; 10·14; 20·13; 40·8; 00·15; 50·11; 30·12; 20·14; 21·11; 50·2; 31·11; and 32·8; the intensity was so small that the spacing was not determined.

[7] Hull and Davey, Phys. Rev. **17**, 549 (1921)

TABLE XIII

Summary of results for the purest samples

Metal	Purity (percent)	Lattice constant a ($\times 10^{-8}$ cm)	Closest atomic approach ($\times 10^{-8}$ cm)	Density from x-ray data	Density from literature[8]
Al	99.97	$4.046 \pm .004$	$2.860 \pm .003$	$2.688 \pm .008$	2.708
Fe	99.937	$2.855 \pm .003$	$2.472 \pm .002$	$7.93 \pm .03$	7.8 – 7.9
Ni	99.548	$3.499 \pm .003$	$2.474 \pm .002$	$9.04 \pm .03$	8.6 – 8.93
Cu	99.99	$3.597 \pm .004$	$2.543 \pm .003$	$9.01 \pm .03$	8.91 – 8.96
Mo	99.8	$3.142 \pm .003$	$2.720 \pm .003$	$10.21 \pm .03$	8.6 – 9.1
Pd	"Heraeus"	$3.859 \pm .004$	$2.729 \pm .003$	$12.25 \pm .04$	11.4 – 11.9
Ag	99.999	$4.079 \pm .004$	$2.884 \pm .003$	$10.49 \pm .03$	10.50 – 10.53
W	99.999	$3.155 \pm .001$	$2.732 \pm .001$	$19.32 \pm .02$	18.77
Pt	99.995	$3.912 \pm .004$	$2.766 \pm .003$	$21.51 \pm .06$	21.16 – 21.50
Au	99.999	$4.065 \pm .004$	$2.874 \pm .003$	$19.37 \pm .06$	19.27 – 19.32
Pb	99.96?	$4.920 \pm .005$	$3.479 \pm .003$	$11.48 \pm .03$	11.34
Bi	crystal	$4.539 \pm .005$ (hexagonal axes) (axial ratio = 2.606)		$9.80 \pm .03$	9.75 – 9.80

It is a pleasure to express my thanks to Dr. G. Breit of the Laboratory of Terrestrial Magnetism, Carnegie Institution, for supplying me with pure specimens of Fe, Cu, Ag, Pt, and Au, together with a statement of the original source and purity of each; and to J. D. Edwards of the Aluminum Co. of America, W. L. Enfield, G. E. Inman, and Dr. W. E. Forsythe of the Nela Laboratories, and Dr. R. W. Moore, Dr. S. L. Hoyt, Dr. D. H. Brophy, and T. S. Fuller of this laboratory for supplying other specimens and for giving statements of their purity; and to Mrs. J. L. Leudemann for assistance in preparing the specimens and reading the diffraction patterns.

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[8] From Van Nostrand's Chemical Annual and from Groth's Chemische Krystallographie.