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Thermophysical Properties of Some Key Solids[1]

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In 1985 the Committee on Data for Science and Technology (CODATA) published a Report of its Task Group on Thermophysical Properties of Solids which analyzed available data on, and gave recommended values for, the heat capacity of Al_2O_3, Cu, W, and Fe, the thermal expansion of Cu, Si, W, and Al_2O_3, the electrical resistivity of Cu, Fe, W, and Pt, the thermal conductivity of Al, Cu, Fe, and W, and the absolute thermopower of Pb, Cu, and Pt. The Chairman of the Task Group was Professor Y. S. Touloukian, until his death in 1981, and later was Dr. Merrill Minges. Since that publication there have been more measurements of heat capacity (Cu), thermal expansion (Si and W), and thermopower (W), particularly at high temperatures with subsecond techniques, which have led us to reanalyze some of the data and change some "recommended" values. Revised tables and some algebraic expressions are presented here.

KEY WORDS: absolute thermopower; evaluated data; electrical resistivity; heat capacity; thermal conductivity; thermal expansion; Al_2O_3; Cu; Fe; Pt; Si; Pb; W.

1. INTRODUCTION

In 1974, the Committee on Data for Science and Technology (CODATA), a member of the International Council of Scientific Unions (ICSU), established a Task Group on Transport Properties which was charged with promoting the availability of reliable reference data on the transport properties of solids [1]. This group was chaired by the late Professor Y. S. Touloukian of Purdue University and later broadened its scope from

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"transport" to "thermophysical" properties. Professor Touloukian was succeeded as Chairman by Dr. Merrill Minges (Wright-Patterson Laboratories) until the publication of the report [2] entitled "Thermophysical Properties of Some Key Solids" as a CODATA Bulletin in 1985, after which the Task Group was dissolved. Other members of the group were Alan Beck (University of Western Ontario), Robert Berman (Oxford University), Francois Cabannes (University d'Orleans), Jerry Hust (NBS Laboratories at Boulder), and Guy White (Sydney).

The purpose of the report [2] was to produce a set of recommended values for some important thermal and electrical properties of solid materials which are used for checking and calibrating measuring equipment. The materials (including copper, alumina, tungsten, platinum) were chosen not necessarily because they were nationally certified reference materials (such as SRMs in the United States) but rather because they satisfied the criteria of availability in stable and well-characterized form as well having extensive property data in the literature. Apart from members of the Task Group, a number of others who were well versed in particular properties or materials acted as analysts (see list in Ref. 2). Their task was to examine the best available data and produce (i) tables of mean values with estimates of uncertainties, (ii) plots of deviations of the treated data from the mean values, and (iii) algebraic representations where possible. The reports from the analysts were reviewed and abbreviated to appear in the 1985 CODATA bulletin.

Since that bulletin appeared, there have been further measurements (chiefly in national laboratories) and critical evaluations of the heat capacity of copper [3, 4], thermal expansion of silicon [5] and tungsten [6], and thermopower of tungsten [7]. This had led us [8] to update and amend some sections of the bulletin. The present brief report is intended to draw attention to the 1985 CODATA Bulletin and indicate the changes in "recommended" values resulting from reanalysis with newer data.

Before considering the different properties it seems important to emphasize the differing effects produced by trace impurities. For heat capacity and thermal expansion, minor traces (say ~ 0.1 at %) have little effect except at the lowest temperatures, where the lattice energy is very small. However, the transport properties (electrical resistivity, ρ; thermal conductivity, λ; thermal diffusivity, D; and thermopower, S) are dominated by impurity scattering or grain size at low temperatures and these can be important at intermediate temperatures. For example, a change from 1- to 2-ppm impurity in copper will alter ρ by a factor of two at the lowest temperatures but may be undetectable in the heat capacity.

2. HEAT CAPACITY OF α-Al_2O_3, Cu, W, AND Fe

Table I gives the recommended values of the heat capacity at constant pressure, C_p, for these four solids, incorporating changes from Ref. 2 in the case of Cu and W. Values at constant volume, C_v (see Refs. 2 and 8) are omitted in the present paper for reasons of space.

For alumina, the values are from the detailed analysis by Castanet [9] and differ by less than 0.5% from those for the SRM 720 of NBS (now NIST) [10] from 20 to 1200 K and $\leqslant 1$% from 1200 to 2000 K. The more recent IUPAC evaluation [4] agrees closely with Table I below 1300 K, differences reaching 1% at 1600 K. Note that Archer [11] has reanalyzed the thermodynamic properties of SRM 720 and the effect of temperature-scale differences. His values of C_p agree with the present Castanet values within 0.2% above 200 K and within 0.4% below this.

For copper, the tabulated values from 30 to 300 K are taken from the polynomial recommended by IUPAC [4] and lie within 0.2% of Martin's data [3]. Above 300 K we have continued to use the values recommended by Hultgren *et al.* [12]. The deviation plot in Fig. 1 also includes recent high temperature values, denoted "Do" [13].

For tungsten, the CODATA values [2] prepared by White and Collocott [14] have been amended slightly at high temperatures with the

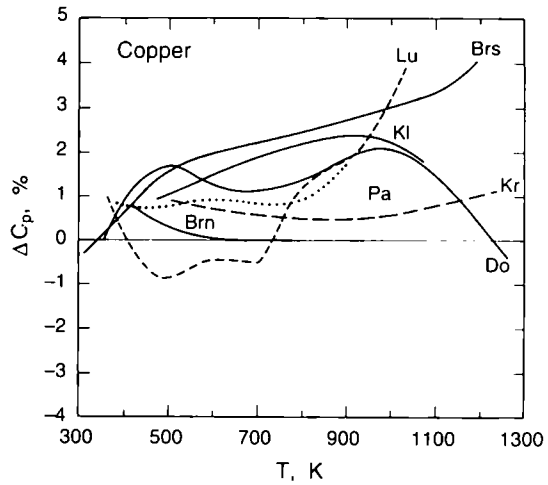

Fig. 1. Copper. Deviation of C_p data from recommended values in Table I between 300 and 1300 K. For symbols see text and Ref. 14.

Table I. Heat Capacity C_p ($J \cdot mol^{-1} \cdot K^{-1}$)

T (K)	Al_2O_3	Cu	W	Fe
10	0.0087	0.0554	0.045	0.068
20	0.073	0.462	0.333	0.25
30	0.263	1.688	1.35	0.74
40	0.698	3.725	3.30	1.66
50	1.506	6.162	5.82	3.01
60	2.793	8.62	8.39	4.76
70	4.594	10.89	10.74	6.69
80	6.902	12.87	12.81	8.64
90	9.677	14.56	14.57	10.45
100	12.85	16.00	16.04	12.05
120	20.07	18.26	18.28	14.92
140	27.94	19.86	19.87	17.18
160	36.04	21.03	21.01	19.00
180	43.91	21.90	21.86	20.32
200	51.33	22.58	22.51	21.46
250	67.17	23.74	23.65	23.57
273.15	73.22	24.13	23.98	24.25
300	79.64	24.44	24.35	25.02
350	88.91	24.88	24.69	26.19
400	96.08	25.25	24.92	27.36
500	106.13	25.91	25.38	29.71
600	112.55	26.48	25.83	32.05
700	116.92	26.99	26.25	34.60
800	120.14	27.48	26.24	37.95
900	122.81	28.04	27.03	43.10
1000	125.02	28.66	27.39	54.43
1100	126.79	29.48	27.76	46.40
1200	128.25	30.53	28.12	34.01
1300	129.22		28.48	34.85
1400	130.16		28.85	35.69
1500	131.0		29.24	36.53
1600	132.1		29.67	37.36
1700	133.2		30.10	41.46
1800	134.4		30.57	
2000	137.0		31.66	
2200	139.7		32.96	
2400			34.53	
2600			36.42	
2800			38.68	
3000			41.36	
3200			44.52	
3400			48.21	

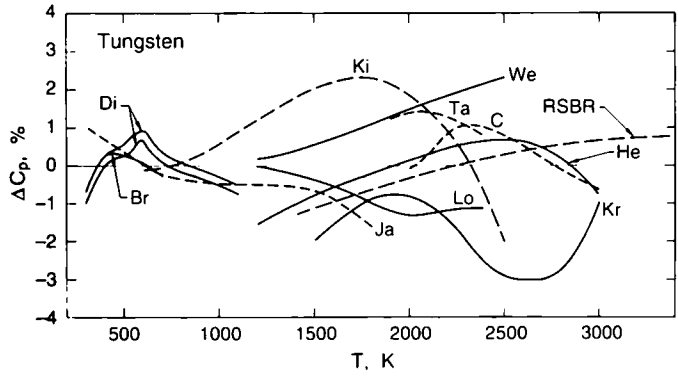

Fig. 2. Tungsten. Deviation of C_p data from recommended values in Table I from 300 to 3500 K [19]. For symbols see text and Ref. 14.

incorporation of recent measurements of Righini *et al.* [15] from 1500 to 3600 K (see "RSBR" in Fig. 2). The amended polynomial to fit data from 300 to 3500 K is $C_p = \sum A_n t^n$ J · mol^{-1} · K^{-1}, where $t = T/1000$ and

$$A_{-1} = 0.1406637, \qquad A_1 = 8.068661, \qquad A_3 = 1.075862$$

$$A_0 = 21.868372, \qquad A_2 = -3.756196$$

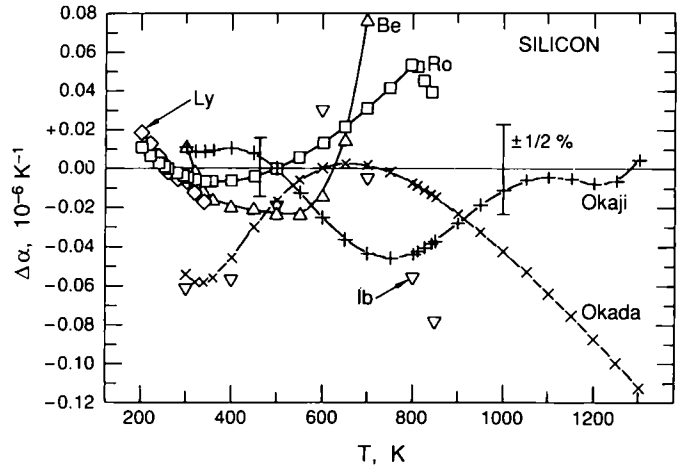

Fig. 3. Silicon. Deviation of α-values from polynomial fit. For symbols see text and Ref. 18.

Iron was included because of its importance as a thermal conductivity and diffusivity standard rather than for its heat capacity. The values are complicated because of the ferromagnetic transition at 1043 K and crystallographic changes at 1185 and 1667 K. Current values in Table I are those from the CODATA Bulletin [2] and based on Hultgren *et al.* [12]. A later analysis by Desai [16] recommends values from 298 to 1800 K which differ by less than 1% from these except in the vicinity of the transitions.

3. THERMAL EXPANSION OF Cu, Si, W, AND α-Al_2O_3

As emphasized at the 11th Symposium on Thermophysical Properties [17] in a paper entitled "Reference Materials for Thermal Expansion," significant errors can occur in dilatometry, particularly with push-rod systems, unless calibrations are done with well-characterized materials. Recommended values of the linear coefficient, $\alpha^* = (1/l_T)\, dl/dT$ (summarized in Table II), are similar to those in Ref. 17, which also includes the integrated length changes, $\Delta l/l_{293}$, omitted here for space reasons.

Differences here and in Ref. 17 from the CODATA values [2] occur at high temperatures for Si and W. The reanalysis for Si by Swenson [18] now incorporates measurements at NRLM, Japan [5], and that for W includes the NIST data [6].

For Si, Swenson has fitted the data to the reference function (90–1300 K):

$$\alpha^* = -0.713 + 5.04x^2e^x/(e^x - 1)^2 + 0.180(y - 1)^2/(1 + 0.36y) \qquad (1)$$

where α^* is in $10^{-6}\,K^{-1}$, $x = 685/T$, $y = T/435$, and T is in K.

For W, Roberts [19] has fitted to the following polynomial for the range 300–3500 K (using $t = T/1000$):

$$\alpha^* = 3.873 + 2.562t - 2.8613t^2 + 1.9862t^3 - 0.58608t^4 + 0.070586t^5 \qquad (2)$$

where α^* is in $10^{-6}\,K^{-1}$.

In Refs. 2 and 17 polynomial expressions are given for Cu and for polycrystalline alumina at temperatures above 300 K. These fuller treatments tabulate the principal linear coefficients, $\alpha_{\parallel}$ and $\alpha_{\perp}$, for single crystal alumina up to 1000 K.

Table II. Values of $\alpha^* = (1/l_r)\,dl/dT$ ($10^{-6}\,K^{-1}$)

T (K)	Cu	Si	W	Al_2O_3 (av.)
10	0.030	0.0005	0.006	
15	0.103	0.0012	0.019	
20	0.263	−0.003	0.048	0.004
25	0.56	−0.019	0.102	0.009
30	1.00	−0.053	0.20	0.016
40	2.27	−0.164	0.53	0.054
50	3.84	−0.29	0.96	0.120
60	5.46	−0.40	1.43	0.18
70	6.98	−0.46	1.88	0.29
80	8.33	−0.47	2.30	0.44
90	9.49	−0.43	2.61	0.61
100	10.49	−0.34	2.88	0.81
120	12.05	−0.06	3.30	1.28
140	13.19	0.31	3.59	1.80
160	14.03	0.69	3.81	2.34
180	14.67	1.06	3.97	2.90
200	15.19	1.40	4.10	3.42
250	16.11	2.10	4.30	4.52
293	16.65	2.56	4.42	5.30
300	16.70	2.62	4.43	5.40
350	17.12	2.99	4.48	6.08
400	17.51	3.26	4.55	6.64
500	18.23	3.61	4.65	7.46
600	18.93	3.83	4.74	7.99
700	19.67	4.00	4.82	8.35
800	20.46	4.11	4.89	8.62
900	21.32	4.21	4.97	8.86
1000	22.26	4.30	5.05	9.09
1100	23.31	4.39	5.13	9.34
1200	24.58	4.47	5.22	9.59
1300		4.56	5.32	9.85
1400			5.43	10.09
1500			5.55	10.31
1600			5.68	10.51
1700			5.83	10.67
1800			5.98	10.84
2000			6.32	11.37
2200			6.72	
2400			7.18	
2600			7.71	
2800			8.34	
3000			9.12	
3200			10.09	
3400			11.33	

4. ELECTRICAL RESISTIVITY OF Cu, Fe, Pt, AND W

We have not amended the chosen values of "ideal" resistivity, ρ_i, tabulated in the earlier bulletin [2] together with some polynomial fits. The major sources of the chosen values were as follows: for Cu, the evaluation of Matula [20] (see also Bass [21]); for Fe, that of Chu and Ho [22]; for Pt, that of White [23]; and for W, that of Chu and Ho [22].

5. THERMAL CONDUCTIVITY OF Al, Cu, Fe, AND W

The values in the bulletin [2] were prepared by J. G. Hust and based on the detailed NBS Internal Report by Hust and Lankford [24]. They collated the principal measurements of thermal conductivity of these four elements from 1 K to the melting point, correlated them with partly empirical expressions, and used resulting functions to generate tables and graphs of conductivity as a function of temperature and "electrical purity" or residual resistance.

6. ABSOLUTE THERMOPOWER OF Pb, Cu, Pt, AND W

To find the absolute thermoelectric power S of a material (A), it is necessary to measure the Thomson coefficient, μ, from 0 K up to the temperature of interest, then $S(T) = \int_0^T (\mu/T)\, dT$. The Thomson heat is the heat absorbed (or produced) when electrons flow along a temperature gradient in the material and it can be measured from the change in temperature profile of a rod when the current direction is reversed. This is not easy to do with accuracy as the Thomson heat is small compared with the Joule heating. Once the thermopower S_A is measured, then that of another material (B) can be found more easily by measuring the differential thermopower of the pair, S_{AB}. Thence $S_B = S_{AB} + S_A$.

Most values of S quoted prior to 1977 traced their origin back to measurements and intercomparisons done by Borelius and his group between 1910 and 1932 [25] and later by Nystrom [26] and Lander [27]. Since then Roberts measured μ for Pb [28], then extended these with Cu up to 900 K [29]. Finally, he and colleagues [7] measured Pt and W from 900 to 1700 K. The results are in Table III. Note that the CODATA Bulletin [2] did not include the tungsten values.

Table III. Absolute Thermopower, S ($\mu V \cdot K^{-1}$) for Pb, Cu, Pt, and W

T (K)	S (Pb)
0.0	0.000
7.2(s)[a]	0.000
7.2(n)[b]	−0.200
7.5	−0.220
8.0	−0.256
9.0	−0.343
9.5	−0.388
10.0	−0.433
10.5	−0.476
11.0	−0.517
11.5	−0.556
12.0	−0.593
13.0	−0.657
14.0	−0.707
15.0	−0.745
16.0	−0.770
17.0	−0.782
18.0	−0.786
20.0	−0.779
22.0	−0.760
24.0	−0.735
26.0	−0.707
28.0	−0.681
30	−0.657
32	−0.636
34	−0.617
36	−0.601
38	−0.587
40	−0.575
45	−0.551
50	−0.537
55	−0.530
60	−0.527
70	−0.531
80	−0.544
90	−0.562
100	−0.583
120	−0.631
140	−0.682
160	−0.734
180	−0.785
200	−0.834
220	−0.882
240	−0.927
260	−0.969

Table III. *(Continued)*

T (K)	S (Pb)	S (Cu)	S (Pt)	S (W)
273	−1.00	1.79	−4.04	0.77
300	−1.05	1.94	−4.92	1.44
350	−1.16	2.22	−6.33	2.95
400	−1.28	2.50	−7.53	4.62
450	−1.41	2.78	−8.59	6.26
500	−1.56	3.07	−9.53	7.85
550	−1.73	3.35	−10.41	9.34
600		3.62	−11.22	10.75
650		3.89	−11.98	12.08
700		4.16	−12.71	13.33
750		4.43	−13.42	14.48
800		4.70	−14.14	15.51
850		4.96	−14.89	16.40
900		5.23	−15.66	17.19
1000			−17.21	18.46
1100			−18.77	19.40
1200			−20.29	20.06
1300			−21.78	20.45
1400			−23.18	20.63
1500			−24.49	20.70
1600			−25.67	20.61
1700				20.12
1800				19.15

[a] Superconducting.
[b] Normal.

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