Checks and estimates for material properties
I. Ranges and simple correlations

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Material properties of solids have values which—for a given structure and bond-type (defining a 'class' of solid)—lie within broadly defined *ranges*, characteristic of the class. Beyond this, *correlations* exist between the values of mechanical, thermal, electrical and other properties which derive from the underlying physics of bonding and packing of atoms in the material. Some of these correlations have a simple theoretical basis and can be expressed as *dimensionless groups* with much narrower value ranges; they allow a physically based consistency check on property values and allow some properties to be estimated when values for others are known. Others, empirical at this stage, can be found by an appropriate search routine; they, too, can be used to estimate missing properties, and to assign a reliability range to the estimates.

The results are useful whenever calculations involving material properties are undertaken. They allow the detection of errors in the values of material properties which are used as inputs to the calculations; and they permit calculations to proceed even when some data are missing by providing intelligent estimates for the missing values. This paper assembles property ranges and dimensionless correlation-groups for commonly used properties, examines their accuracy and illustrates their utility. A companion paper develops and illustrates the empirical-correlation method.

Keywords: material data estimation; material data validation; property correlations

1. Introduction

(*a*) *Material properties, material classes and property correlations*

The properties of solids derive ultimately from the way in which the atoms or molecules are arranged in space (*structure*) and the nature of the intermolecular forces that hold them together (*bonding*). From this follows the two lines of arguement on which this paper relies. The first: that materials with similar structure and bonding (defining a *material class*) exhibit similarities in their properties—their values lie within defined ranges, characteristic of their class. The second: that since all properties ultimately derive from structure and bond type, the properties of a material are, to varying degrees, interrelated; these relationships can be expressed as dimensionless property groups with values which, for a given class of material, can be almost constant.

To elaborate a little: materials, commonly, are classified as *metals*, *polymers*, *elastomers*, *ceramics* and *glasses*; to these we must add the wide range of *composites*

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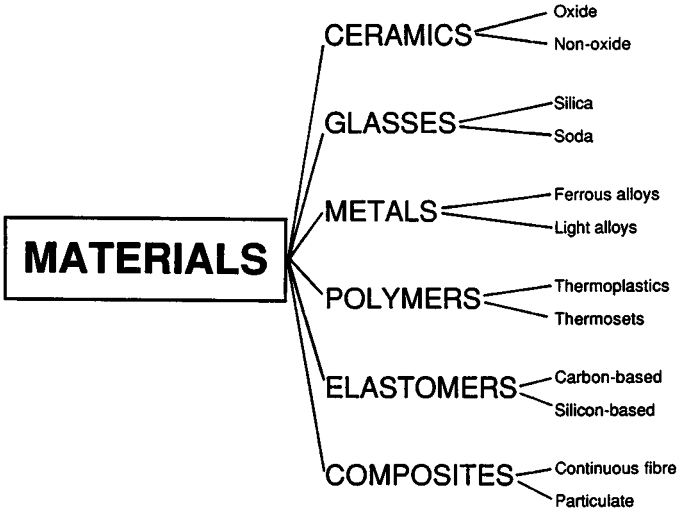

Figure 1. Material classes and subclasses. Only two subclasses are shown for each class; each, in reality, has many.

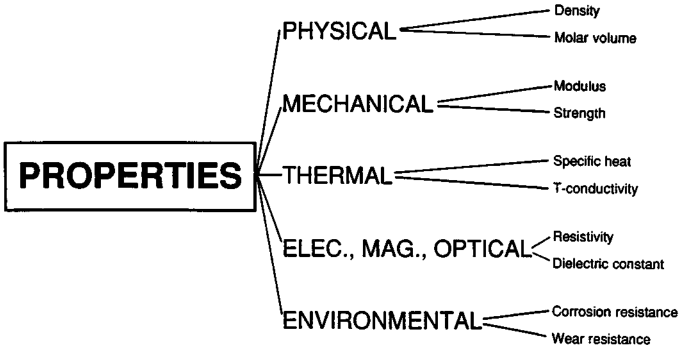

Figure 2. Material properties. Each property type has many members, of which only two are shown.

which can be made by combining them (figure 1). Each class has a number of subclasses: ferrous alloys, light alloys and refractory metals within the class of metals, for instance, or thermoplastics and thermosets within that of polymers. And these can be subdivided further: cast irons, carbon steels, low- and high-alloy steels within the subclass of ferrous alloys, for instance. Within a class or subclass there exists a certain commonality of properties; between them there is usually a contrast. Metals as a class are stiff and good electrical conductors, polymers as a class are neither; ceramics as a class are hard and brittle, elastomers as a class are the opposite. By 'properties' we mean not just the physical, mechanical, thermal, electrical and magnetic characteristics of a material, but also measures of their interaction with their environment: oxidation, corrosion, wear and other such (figure 2). Put succinctly: properties for a material class or subclass have *characteristic ranges of values*, explored in § 2.

Beyond this, *correlations* exist between certain properties. Correlations are strongest between properties which derive in a direct way from the nature of the atomic bonding and structure—the strong correlation between modulus and the melting point or that between specific heat and density are examples. The correlations are less strong (but still useful) when they derive from properties which depend on defects in the structure—strength and toughness, for instance. They are weakest when interaction with the environment is involved; i.e. in describing corrosion, wear and suchlike. The correlations can often be expressed as *limits for the values of physically based dimensionless property groups*, developed in § 3.

(*b*) *The checking and estimation of material property data*†

Materials-related calculations, models and simulations require, as inputs, data for the properties of materials. Examples of such activities are the numerical calculation of the service response of a component to mechanical or thermal loads, the modelling the structural evolution of the material itself during processing, and the selection of materials for engineering design. The data are important: the quality of the output can never be better than that of the input; and missing data can disable the calculation completely. The value of a database of material properties depends on its precision and its completeness, in short, on its quality.

One way of maintaining or enhancing quality is to subject data to validating procedures. The property ranges and dimensionless correlations provide powerful tools for doing this. The same procedures fill a second function: that of providing estimates for missing data, essential when no direct measurements are available. The method can be thought of as introducing a degree of 'intelligence' into the database; the correlations encapsulate knowledge unfamiliar to the operator, called and used in appropriate ways in which the operator need not be expert, yet furthering his goals.

(*c*) *Empirical correlations*

Property ranges can be listed for all material classes and properties; but well-established, physically based, correlations relate only some of them. When no simple correlation is known, it is still possible to hunt, with an appropriate search routine, for empirical links, and base an estimation procedure on those. This approach is developed in a companion paper (Bassetti *et al.* 1998).

2. Property ranges

(*a*) *Range checks: monolithic materials*

Trivial though it may seem, it is valuable, when creating a database, to tabulate the known range of values of each material property for each class in the database, and check whether each new datum lies within the appropriate range. A convenient way of presenting the information is as a table in which a low (L) and a high (H) value are stored, identified by the material class. An example, listing Young's modulus, E, for a representative set of material classes, is shown in table 1, in which E_{L} is the lower limit and E_{H} the upper limit. Table 2 lists ranges for the engineering properties of one subclass of metals, that of *ferrous alloys*; it includes cast irons, carbon, low- and high-alloy steels.

Figure 3 shows one of these properties, the thermal expansion coefficient, α, plotted as a bar-chart. It illustrates that the property range for a class, though wide, is much narrower than the spread of the value of properties for *all* materials; that is why it is useful to associate property ranges with a class. All properties have characteristic ranges like these. The use of the ranges for property checking is obvious: any new

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† The method has been used for some years in the author's laboratory (examples are contained in the HIP software (1980), the T-maps software (1986) and the CMS 2.0 software (1995)).

Table 1. *Ranges of Young's modulus E for broad material classes*

material class	E_L (GPa)	E_H (GPa)
all solids	0.00001	1000
classes of solid		
metals: ferrous	70	220
metals: non-ferrous	4.6	570
fine ceramics[a]	91	1000
glasses	47	83
polymers: thermoplastic	0.1	4.1
polymers: thermosets	2.5	10
polymers: elastomers	0.0005	0.1
polymeric foams	0.00001	2
composites: metal–matrix	81	180
composites: polymer–matrix	2.5	240
woods: parallel to grain	1.8	34
woods: perpendicular to grain	0.1	18

[a] Fine ceramics are dense monolithic ceramics such as SiC, Al_2O_3, ZrO_2, etc.

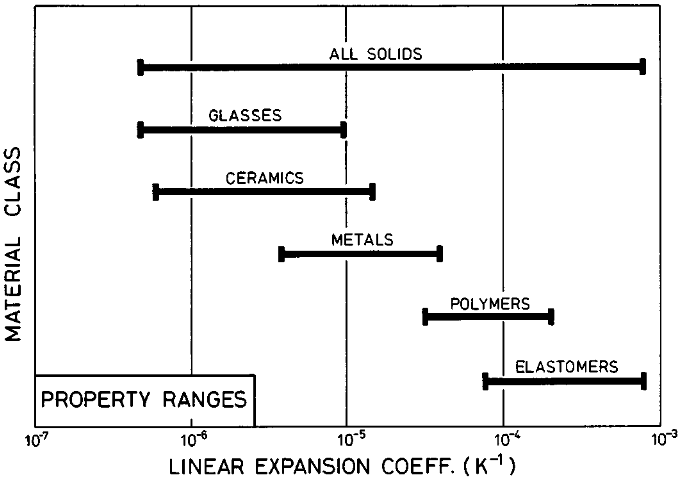

Figure 3. A bar chart showing the range of values of expansion coefficient, α, for generic material classes. The range for all materials spans a factor of almost 3000. That for a class spans, typically, a factor of 20.

datum should lie in its proper band of figure 3 or its equivalents for other properties; if it does not, it should be checked.

The method becomes more discriminating if the classes are narrower. We have found that, in dealing with metals, separating the ranges for cast irons, steels, aluminium alloys, magnesium alloys, titanium alloys, copper alloys, etc., is practical and works well. Similar subdivisions for polymers (thermoplastics, thermosets, elastomers) and for ceramics and glasses (engineering ceramics, whiteware, silicate glasses, minerals) increases resolution here also. The low and high values are not absolute limits: occasional properties of idiosyncratic materials (like beryllium among metals,

Table 2. *Ranges for engineering properties for the class 'ferrous alloys'*
('Ferrous alloys' includes cast-irons, carbon steels, low- and high-alloy steels.)

property	units	P_L	P_H
general physical properties			
atomic volume, V_m	$m^3\ kmol^{-1}$	0.0069	0.0082
density, ρ	$kg\ m^{-3}$	6900	8100
mechanical properties			
bulk modulus, K	GPa	50	117
Young's modulus, E	GPa	70	220
shear modulus, G	GPa	27	87
Poisson's ratio, ν	—	0.25	0.30
compressive strength, σ_c	MPa	111	2250
elastic limit, σ_y	MPa	65	2250
modulus of rupture, σ_{MOR}	MPa	75	2250
tensile strength, σ_{ts}	MPa	90	2240
endurance limit (fatigue), σ_e	MPa	40	800
hardness, H	MPa	900	7600
ductility (elongation), ε_f	—	0.002	0.7
fracture toughness, K_{Ic}	$MPa\ m^{1/2}$	9	150
loss coefficient, η	—	0.0002	0.035
thermal properties			
melting point, T_m	K	1403	1803
maximum use temperature, T_{max}	K	420	1500
minimum use temperature, T_{min}	K	1	250
specific heat, C_p	$kJ\ kg^{-1}\ K^{-1}$	265	560
latent heat of fusion, L_m	$kJ\ kg^{-1}$	260	285
thermal conductivity, λ	$W\ m^{-1}\ K^{-1}$	11	72
expansion coefficient, α	$10^{-6}\ K^{-1}$	8	20
electrical properties			
electrical resistivity, R	$10^{-8}\ \Omega\ m$	15	120

or ice among ceramics) may lie outside them. The limits define the range within which it is very probable (greater than 95% confidence) that a property will lie, for reasons given shortly.

3. Dimensionless property groups

(*a*) *Dimensionless correlations between material properties*

Materials which are stiff have high melting points. Solids with low densities have high specific heats. Metals with high thermal conductivities have high electrical conductivities. These rules-of-thumb describe correlations between two or more material properties which can be expressed more quantitatively as limits for the values of

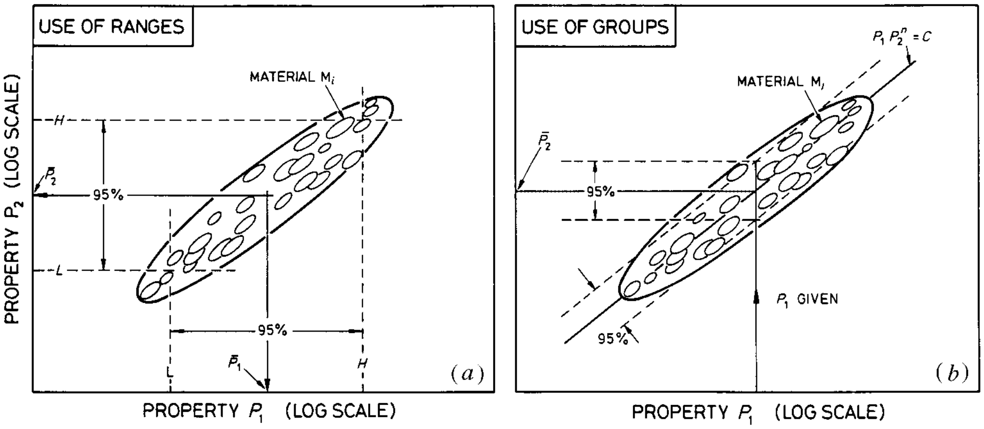

Figure 4. (*a*) The use of the property ranges to check and estimate data; and (*b*) the use of correlation to do the same thing, showing the greatly increased precision.

dimensionless property groups. They take the form

$$C_L < P_1 P_2^n < C_H \tag{3.1}$$

or

$$C_L < P_1 P_2^n P_3^m < C_H \tag{3.2}$$

(or larger groupings) where P_1, P_2, P_3 are material properties, n and m are simple powers (usually -1, $-\frac{1}{2}$, $\frac{1}{2}$ or 1), and C_L and C_H are dimensionless constants; the lower and upper limits between which the values of the property group lies. When such correlations exist they permit checks and estimates which are much more discriminating and precise than do the range checks (figure 4).

There is nothing arbitrary in this. Properties of solids derive, ultimately, from the ways in which their atoms or molecules pack and from the nature of the bonds which link them. Some properties—density, moduli, expansion coefficients, specific heat—relate directly to these. Others, those involving defects such as vacancies, dislocations, boundaries or cracks, are still related, but at one or more removes, so to speak; correlations exist here too, though their limits are wider. When the environment is involved, as it is in corrosion and wear, the correlations become fuzzier still. This perception is not new; there are many catalogues of them (see, for example, Beaman 1952; Davies 1976; Brown & Ashby 1980*a*, *b*; Frost & Ashby 1982; Sammis *et al.* 1981; Fisher 1988). Here we examine those involving the macroscopic mechanical and thermal properties.

An example is the relationship between expansion coefficient, α (K^{-1}), and the melting point, T_m (K) or, for amorphous materials, the glass temperature T_g:

$$C_L \leqslant \alpha T_m \leqslant C_H; \tag{3.3}$$

a correlation with the form of equation (3.1). Values for the dimensionless limits C_L and C_H for this group are listed in table 3 for representative material subclasses. Like those for properties, they are chosen to contain 95% of the data. The limits can be displayed as bar charts, of which figure 5 is an example: it shows the ranges for αT_m for the generic material classes.

The values span a range which is much narrower than that of the properties themselves (table 1). They allow a tighter check on properties and an estimate of one

Table 3. *Limits for the group αT_m and αT_g for broad material classes*[a]

correlation[a] $C_L < \alpha T_m < C_H$	C_L ($\times 10^{-3}$)	C_H ($\times 10^{-3}$)
all solids	0.1	56
classes of solid		
metals: ferrous	13	27
metals: non-ferrous	2	21
fine ceramics*	6	24
glasses	0.3	3
polymers: thermoplastic	18	35
polymers: thermosets	11	41
polymers: elastomers	35	56
polymeric foams	16	37
composites: metal–matrix	10	20
composites: polymer–matrix	0.1	10
woods: parallel to grain	2	4
woods: perpendicular to grain	6	17

[a] For amorphous solids the melting point, T_m is replaced by the glass temperature, T_g.

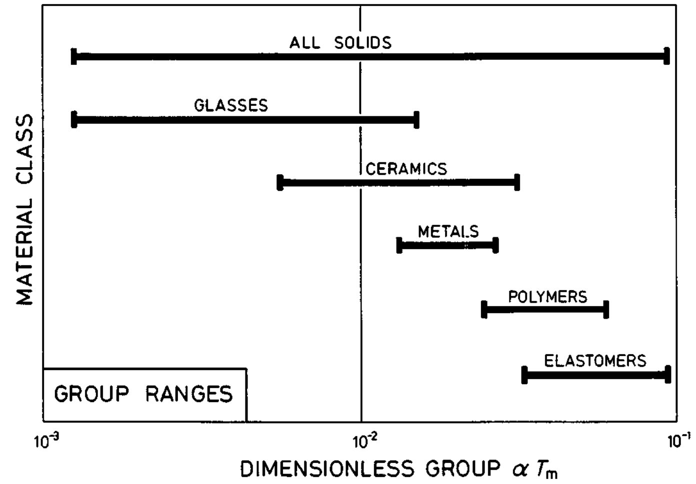

Figure 5. A bar chart showing the range of the dimensionless group αT_m for generic material classes.

property (α, say) when others (T_m in this instance) are known. There are many such correlations. In this paper we limit discussion to those which relate the engineering properties listed in table 2. Others exist which relate surface properties, the properties of solid solutions, liquids and vapours, microscopic properties (such as the energy to form or move a vacancy or interstitial) and the temperature and pressure-dependencies of all of these (Mott & Jones 1936; Kittel 1968; Tabor 1969; Cottrell 1955, 1964; Kelly & Macmillan 1986). Even with this limitation, table 2 generates 22 correlations, documented in the Appendix and listed in the first column of table 4,

Table 4. *Limits for dimensionless property groups for ferrous alloys*

(N_0, Avogadro's number, 6.023×10^{26} kmol^{-1}; R, gas constant, 8.314 kJ kmol^{-1} K^{-1}; b, $(V_m/N_0)^{1/3}$.)

property group	equation	C_L	C_H
G/E	(A 2)	0.36	0.4
K/E	(A 3)	0.69	0.76
KV_m/RT_m or T_g	(A 4)	40	77
EV_m/RT_m or T_g	(A 5)	54	102
$C_p\rho V_m/R$	(A 6)	2.5	3.3
$C_p\rho T_m/K$ or T_g	(A 7)	0.037	0.045
$K_\alpha/C_p\rho$	(A 8)	0.25	0.61
αT_m $(\times 10^{-3})$ or T_g	(A 9)	13	27
$\lambda/bC_p(E\rho)^{1/2}$	(A 10)	3.3	5.8
$L_m\rho V_m/RT_m$	(A 13)	1.03	1.09
L_m/C_pT_m	(A 14)	3.2	3.7
$L_m\rho/K$	(A 15)	0.013	0.015
T_g/T_m	(A 16)	—	—
σ_y/E $(\times 10^{-3})$	(A 17)	0.95	4.4
σ_{ts}/σ_y	(A 18)	1.05	2.0
σ_{ts}/E $(\times 10^{-3})$	(A 19)	1.2	5.6
σ_{MOR}/σ_y	(A 20)	1.0	1.2
σ_c/σ_y	(A 21)	1.02	1.2
H/σ_y	(A 22)	3.6	6.6
σ_c/σ_{ts}	(A 23)	0.4	0.9
$K_{Ic}/\sigma_y\sqrt{b}$	(A 24)	2800	21 200
$K_{Ic}/E\sqrt{b}$	(A 25)	5.25	43.7
G_C/E_b	(A 26)	27.6	1 920

which gives values for C_L and C_H for the subclass *ferrous metals*. The way the groups are used for estimation and checking are described in § 4.

4. Implementation

(*a*) *Data checking*

The method is shown in figure 6. Each datum is associated with a material class, or, at a higher level of checking, with a subclass. It is first compared with the range limits L and H for that class and property. If the property lies within the anticipated range, it is accepted and passes on to the next stage. It if lies outside the range, it is flagged, indicating that its value is exceptional and should be checked. As mentioned earlier, the ranges listed in the table are, deliberately, not absolute—that is, they are chosen such that it is improbable but not impossible (95% confidence) that a datum should lie outside them. The narrower ranges better achieve the goal of catching incorrect values; absolute limits have to be very wide. A flagged datum, then, is not necessarily wrong, but it *is* unusual and merits re-examination; and if, on checking, it is found to be correct it can still be accepted.

Why bother with such low-level stuff? It is because, in computations involving

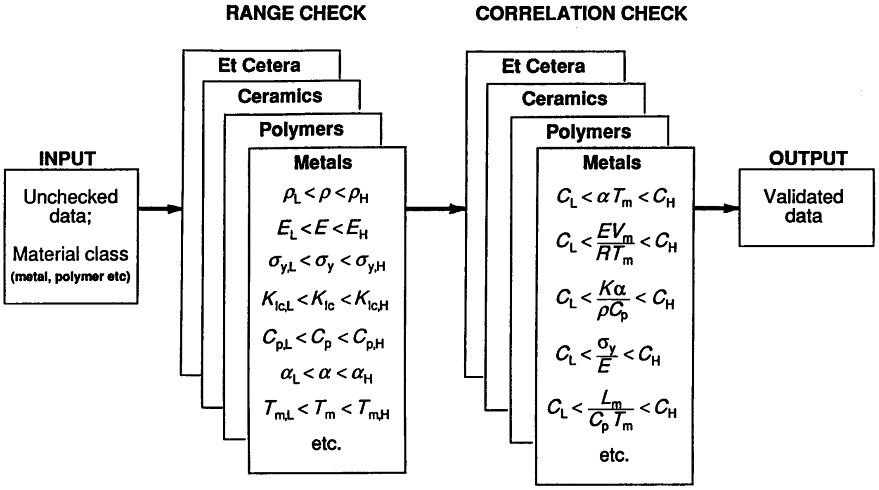

Figure 6. The checking procedure. Range checks catch gross errors in all properties. Checks using dimensionless groups can catch subtler errors in certain properties.

material properties, the commonest error is the use of a property value which is expressed in the wrong units, or is, for less obvious reasons, in error by one or more orders of magnitude (slipped decimal point for instance). Range checks usually catch errors of this sort. If a demonstration of this is needed, it can be found by applying them to the contents of standard reference data books; none among those we have tried has passed without errors. There are better checks, described next, but they cannot be applied to all properties, as these can.

In the second stage, each of the dimensionless groups of properties listed in table 4 are formed in turn and compared with the range bracketed by the limits $C_{\rm L}$ and $C_{\rm H}$ for their class or subclass. If the value lies within its limit-range, it is accepted; if not, it is flagged. As with property-range checks, the limit ranges for the dimensionless combinations are chosen such that most (more than 95%) lie within them; they could be widened to include all known and anticipated values but the narrower ranges make for greater discrimination. If, when checked, a flagged result is found to be correct, it is accepted by the operator who can, if desired, widen the limits to include it if the check were rerun.

(*b*) *Data estimation*

In estimating property values, the procedure is reversed: the dimensionless groups are used first because they are usually the more accurate (figure 7). Each group is re-expressed as a rule explicitly describing the property to be estimated. Thus the group

$$C_{\rm L} \leqslant \alpha T_{\rm m} \leqslant C_{\rm H}, \tag{4.1}$$

gives rise to two rules. The first rule estimates α if $T_{\rm m}$ is known:

$$\frac{C_{\rm L}}{T_{\rm m}} \leqslant \alpha \leqslant \frac{C_{\rm H}}{T_{\rm m}}. \tag{4.2}$$

The second estimates $T_{\rm m}$ if α is available:

$$\frac{C_{\rm L}}{\alpha} \leqslant T_{\rm m} \leqslant \frac{C_{\rm H}}{\alpha}. \tag{4.3}$$

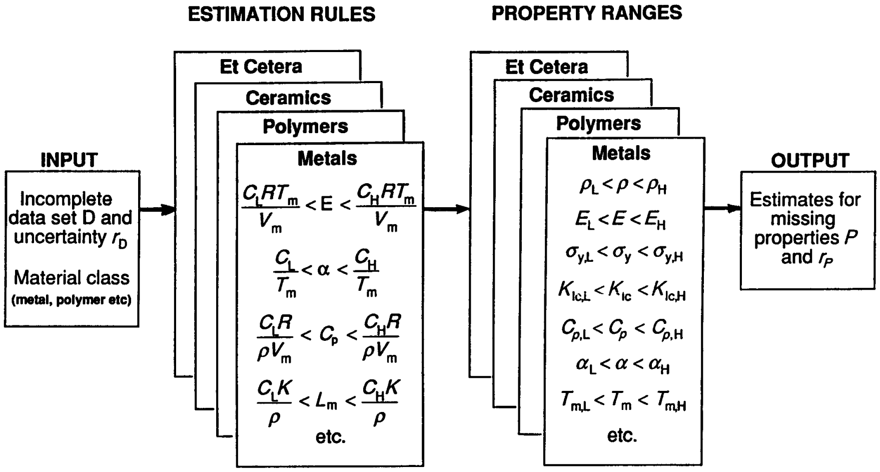

Figure 7. The estimating procedure. The dimensionless groups give rules for estimating one property when others are known. Failing this, the geometric mean of the range provides a first crude estimate. The method also gives a value for the uncertainty in the estimate.

A group such as

$$C_L \leqslant \frac{C_v T_m \rho}{E} \leqslant C_H,$$

generates four rules, one for each of the properties it contains. Each rule R has the form of equation (4.2) or (4.3) which we generalize to

$$R_L \leqslant P \leqslant R_H, \tag{4.4}$$

where P is the property to be estimated and R_L and R_H are the *rule limits.* All the groups listed in the Appendix can be used in this way, giving a portfolio of estimation rules for many, though not all, properties. From these we calculate a *best estimate*, $\bar{P}$, and a *factor of uncertainty*, R_P, for the missing property.

Only when the potential of the correlations is exhausted are the property ranges invoked. They provide a crude first estimate of the value of the missing property, far less accurate than that of the correlations, but still useful as a first guess†. For these, too, we calculate a best estimate and an uncertainty value. The meaning of these words is defined next.

(*c*) *Best estimates, uncertainty and its aggregation*

It is a common observation that the values of material properties, and of the dimensionless groups, are distributed logarithmically, not linearly, within a range. Put another way: a histogram for the the values of a property or group is symmetric when plotted on a logarithmic scale, but not when plotted on a linear one. When the range is narrow the distinction disappears, but when the range is wide—when, for example, it spans a factor of two or more—it becomes important. If the distribution were linear, a best estimate for the property would be the arithmetic mean of the high and low limits of the range (figure 8, left). When it is logarithmic (figure 8, right), the best estimate for the most probable value, $\bar{P}$, for the property P is, instead:

$$\bar{P} = \sqrt{P_L P_H}, \tag{4.5}$$

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† The method described in the companion paper (Bassetti *et al.* 1998) replaces this by a more involved, but more accurate, procedure.

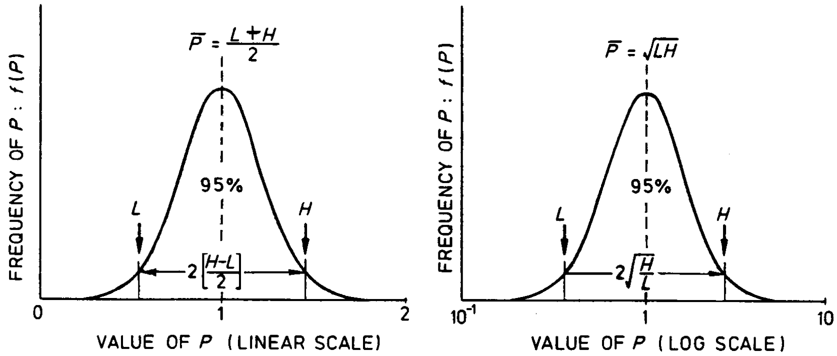

Figure 8. (Left) An expected frequency function for the value of a property or property group, if distributed linearly, the mean and uncertainty are shown. (Right) The same for a property or group with a logarithmic distribution. Properties and groups behave more nearly like the second of these.

where P_{L} and P_{H} are the range limits like those of table 2.

Even the most precise of properties or rules have a margin of uncertainty associated with them. We measure the uncertainty in a property P or a rule R by assigning to it an r-value ('r' stands for 'ratio'). The r-value measures the width of the distribution of P; it is a number greater than one, defined as the ratio of the upper limit for the range divided by the mean:

$$r_P = \frac{P_{\mathrm{H}}}{\sqrt{P_{\mathrm{L}} P_{\mathrm{H}}}} = \sqrt{\frac{P_{\mathrm{H}}}{P_{\mathrm{H}}}}. \tag{4.6}$$

The best estimate and the uncertainty in the value of a property calculated from a rule is found in the same way. Using the generalized form of equation (4.4), the best estimate provided by the rule is

$$\bar{P} = \sqrt{R_{\mathrm{H}} R_{\mathrm{L}}}. \tag{4.7}$$

The uncertainty in a rule is defined in the same way, replacing P_{L} and P_{H} of equation (4.6) by the limits R_{L} and R_{H} of the rule:

$$r_R = \sqrt{\frac{R_{\mathrm{H}}}{R_{\mathrm{L}}}} = \sqrt{\frac{C_{\mathrm{H}}}{C_{\mathrm{L}}}} \tag{4.8}$$

(because the common terms in R_{L} and R_{H} cancel when the ratio is formed). The limits of the range of P are recovered via:

$$P_{\mathrm{L}} = \frac{\bar{P}}{r_R} \tag{4.9}$$

and

$$P_{\mathrm{H}} = \bar{P} r_R. \tag{4.10}$$

The way this works is best illustrated by an example. If the modulus, E, of a material has a mean value of $\bar{E} = 200$ GPa and an r-value of $R_E = 1.1$, then it is taken to mean that the value 'very probably' (95% confidence) falls in the range 200/1.1 and 200 × 1.1, that is, between 182 and 220 GPa, or 200 − 9% to +10%. An r-value of two means the value very probably falls within a factor of two of the mean, that is, in the range 100–400. For precise quantities r is very close to 1.0 and $\pm(r-1)$ is a close approximation to the arithmetic accuracy $\pm(P_{\mathrm{H}} - P_{\mathrm{L}})/(2\bar{P})$. Thus

$r = 1.05$ is the same as -4.8% to $+5\%$, negligibly different from $\pm 5\%$; but when uncertainties are large, the r-value is the only sensible measure.

When properties are estimated from the rules, both the rule R and the properties P_1, P_2, etc., which enter it have uncertainties associated with them. Call these r_R and r_{P_1}, r_{P_2}, etc. It is wrong just to add them to give the uncertainty in the estimate—that would imply that the underlying origins of the uncertainty in the rule and its inputs were coupled such that the extreme values of each occurred simultaneously. A better approximation is that the probability distribution function for the value is log-normal (when the range limits become the 2σ points, where σ is the standard deviation of the distribution) and that the uncertainties are independent. Then the proper measure of the uncertainty in the output is given by:

$$\log(r) = \{(\log r_R)^2 + (\log r_{P_1})^2 + (\log r_{P_2})^2 + \cdots\}^{1/2}. \tag{4.11}$$

We adopt this measure as a sensible compromise.

The procedure in using the rules, then, is as follows. Best estimates for the known properties are substituted into the appropriate rule R, giving two outputs R_{L} and R_{H} (equation (4.4)). A 'best estimate' is formed from these (equation (4.7)). Uncertainty factors for the input properties (equation (4.6)) and for the rule (equation (4.8)) are calculated, and combined using equation (4.11). The high and low limits for the new best estimate for the missing property are recovered from equations (4.9) and (4.10). In practice, a missing property can often be estimated by more than one route. Then the result with the smallest value of uncertainty is selected.

This all sounds much more complicated than it really is. The examples of § 5 will clarify the method.

5. Examples of applications

Applications are of two sorts: in validating data for material properties; and in estimating material properties for poorly characterized materials. Validation, described in § 4 *a*, requires no further comment. The examples which follow illustrate the estimation method. In them, a property is estimated for which a measured value is already known, giving an idea of the efficacy of the method.

(*a*) *The thermal expansion coefficient, α, of PEEK, given its glass temperature, T_{g}*

Polyether ether keytone (PEEK) is a thermosetting polymer. The best correlation here is that of equation (4.1), expressed as the rule of equation (4.2). It relates α to the glass temperature, T_{g}, of the polymer. Table 5 lays out the steps. The first column gives the inputs, the second the rule and the third the outputs. The range C_{L}–C_{H} is that characteristic of the subclass *thermosets* of the class *polymers*. The uncertainty in the rule ($r_R = 1.36$) is much greater than that in the inputs ($r_{T_{\mathrm{g}}} = 1.023$). Equation (4.11) then gives an output, r_α, which is essentially that of the rule. The prediction is within 7% of the experimental value. The r_α value suggests that this is fortuitous; a larger discrepancy is possible.

(*b*) *The heat capacity, C_{p}, of zirconium carbide, given its bulk modulus, K, melting point, T_{m}, and density ρ*

Zirconium carbide is a technical ceramic. Density, melting point, modulus and molecular volume are among the first things that physicists measure for a new compound. It is surprising, at first sight, how much can be inferred from them; the

Table 5. *Estimation of the thermal expansion, α, of PEEK*

inputs	rule	output (K^{-1})	experiment (K^{-1})
class: polymer: thermoset	$\frac{C_\mathrm{L}}{T_\mathrm{g}} \leqslant \alpha \leqslant \frac{C_\mathrm{H}}{T_\mathrm{g}}$	$\bar{\alpha} = 51 \times 10^{-3} \underline{\times} 1.36$	$\alpha = 55 \underline{\times} 10^{-3} \underline{\times} 1.2$
$T_\mathrm{g} = 535 \pm 10$ K	$C_\mathrm{L} = 20 \times 10^{-3}$, $C_\mathrm{H} = 37 \times 10^{-3}$		
$r_{T_\mathrm{g}} = 1.02$	$r_R = \sqrt{C_\mathrm{H}/C_\mathrm{L}} = 1.36$		

Table 6. *Estimation of the heat capacity, C_p, of zirconium carbide, ZrC*

inputs	rule	output ($\mathrm{J\ kg^{-1}\ K^{-1}}$)	experiment ($\mathrm{J\ kg^{-1}\ K^{-1}}$)
class: ceramic: carbide	$\frac{C_\mathrm{L} K}{\rho T_\mathrm{m}} \leqslant C_\mathrm{p} \leqslant \frac{C_\mathrm{H} K}{\rho T_\mathrm{m}}$	$\bar{C}_\mathrm{p} = 390 \underline{\times} 2.2$	$C_\mathrm{p} = 351 \underline{\times} 1.05$
$K = 270 \pm 15$ GPa			
$r_K = 1.08$			
$\rho = 6730 \pm 10\ \mathrm{kg\ m^{-3}}$	$C_\mathrm{L} = 0.024$; $C_\mathrm{H} = 0.046$		
$r_\rho = 1.004$	$r_R = \sqrt{C_\mathrm{H}/C_\mathrm{L}} = 1.92$		
$T_\mathrm{m} = 3410 \pm 8$ K			
$r_{T_\mathrm{m}} = 1.002$			

explanation lies, of course, in the way these quantities characterize bonding and structure. Here (table 6) we need three. They are listed, with r-values, in column 1. Column 2 gives the rule (taken from equation (A 7)). Here we use the rule limits for the subclass carbides from the class of technical ceramics. Column 3 gives the output. This too is a reasonable estimate, within 11% of the experimental value. The r-value suggests that larger descrepancies are possible.

(*c*) *Young's modulus, E, for rhenium, given its melting point T_m*

Rhenium is a refractory metal. Here we use the correlation (A 5), expressed as the rule shown in table 7, with values of C_L and C_H for the subclass *refractory* from the class of metals. Inputs, rule, outputs and comparison with experiment are listed. This is less good: the modulus is underestimated by 31%. This is an example in which the estimate could be useful as a screening exercise seeking materials with high moduli: the estimate is good enough to ensure that rhenium would be included. But if the value of E were critical to the futher exercise, data for it must be sought, or measurements undertaken.

(*d*) *The tensile strength, σ_ts, of PVDF, given its Young's modulus, E*

Polyvinylidene fluoride (PVDF) is a thermoplastic. Equation (A 17) provides the necessary rule. Values for the rule limits, C_L and C_H, for the subclass *thermoplastics*

OK?

Table 7. *Estimation of Young's modulus, E, for rhenium*

inputs	rule	output (GPa)	experiment (GPa)
class: metals: refractory	$\dfrac{C_{\mathrm{L}}RT_{\mathrm{m}}}{V_{\mathrm{m}}} \leqslant E \leqslant \dfrac{C_{\mathrm{H}}RT_{\mathrm{m}}}{V_{\mathrm{m}}}$	$\bar{E} = 321\underline{\times}1.6$	$E = 465\underline{\times}1.05$
$T_{\mathrm{m}} = 3440 \pm 10$ K			
$r_{T_{\mathrm{m}}} = 1.003$	$C_{\mathrm{L}} = 60$; $C_{\mathrm{H}} = 0.046$		
$V_{\mathrm{m}} = 0.009\ \mathrm{m}^3\ \mathrm{kmol}^{-1}$	$r_R = \sqrt{C_{\mathrm{H}}/C_{\mathrm{L}}} = 1.6$		
$r_{V_{\mathrm{m}}} = 1.01$			

Table 8. *Estimation of the tensile strength,* σ_{ts} *, for PVDF*

inputs	rule	output (MPa)	experiment (MPa)
class: polymer: thermoplastic	$C_{\mathrm{L}}E \leqslant \sigma_{\mathrm{ts}} \leqslant C_{\mathrm{H}}E$	$\bar{\sigma}_{\mathrm{y}} = 48\underline{\times}2.8$	$\sigma_{\mathrm{y}} = 50\underline{\times}1.2$
$E = 2000 \pm 1000$ MPa	$C_{\mathrm{L}} = 60$; $C_{\mathrm{H}} = 0.046$		
$r_E = 1.7$	$r_R = \sqrt{C_{\mathrm{H}}/C_{\mathrm{L}}} = 2.2$		

of the class *polymers* are listed in table 8, which shows the steps. The estimate for σ_{ts} is close to the actual measurement, but the uncertainty in both, a factor of more than two, give very wide ranges. Such estimates must be regarded as very approximate, but they may still enable a scoping calculation which would be impossible if no values were available.

6. Summary and conclusions

Solid materials have properties which reflect—some closely, some more remotely—the nature of their atoms, their interatomic bonding and their structure. The range of values of these properties is enormous, spanning many orders of magnitude. But materials, like plants and animals, can be classified, and the finer the classification, the narrower are the characteristic property ranges. And since all properties have their ultimate origin in Schrödinger's equation, so to speak, it is to be expected that relationships should exist between them. Such relationships are known, some empirically, some because they appear in physical models for material response. They can be expressed as dimensionless groups with yet narrower value-ranges. This paper uses class-specific property ranges and ranges for the values of dimensionless groups as the basis of a procedure for checking and estimating material properties.

Data for material properties are a vital input to many materials-based activities: design, selection, modelling, stress analysis are examples. The value of the data is enhanced if they are error checked and corrected; and data-files become more useful if they contain no blanks caused by missing data. The wish to estimate data arises from the need to have values, even if only approximate ones, for evaluating design concepts, for implementing models, and for materials selection; missing data prevent the proper evaluation of a design, impede the implementation of a model, or wrongly eliminate materials from a selection exercise. The techniques described above allow estimates for missing data to be made, and the uncertainty in them to be assessed. Their value derives from their predictive power: if the class to which a material belongs is known, then the accumulated data from other members of that class can be exploited to give a first estimate of missing properties; and if some properties of the material are known with accuracy, others can be estimated from them, with predictable uncertainties.

The methods described here use only part of the accumulated data for a material class in making an estimate (the part captured by the property range or the correlation). It is possible to construct a procedure which exploits *all* the accumulated data for the class. It is described in the companion paper (Bassetti *et al.* 1998).

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Appendix A. The correlations

This Appendix catalogues some of the correlations between the properties of engineering materials, expressing them as dimensionless groups. Most derive from fundamental models for material properties, for which see Mott & Jones (1936), Kittel (1968), Tabor (1969) or Cottrell (1955, 1964) and Kelly & Macmillan (1986); a few are empirical (Fisher 1988). Each is expressed as an inequality with the form of equations (3.1) or (3.2). The limits C_{L} and C_{H} describe the 95% range for the value of the group for a particular material class or subclass. Examples of their values for four material classes are given in table 4.

(*a*) *Atomic weight, A, density, ρ, atomic volume, V_{m}, and atom size, b*

It is frequently necessary, in dealing with material properties, to convert from molar to SI units. The conversion requires a relationship between the (average) molar volume, V_{m}, of an atom in the structure ($\mathrm{m}^3\,\mathrm{kmol}^{-1}$), the (average†) atomic weight ($\mathrm{kg\,kmol}^{-1}$), and density, ρ ($\mathrm{kg\,m}^{-3}$):

$$V_{\mathrm{m}} = \bar{A}/\rho.$$

We approximate the atom diameter, b, by

$$b = \left(\frac{CV_{\mathrm{m}}}{N_0}\right)^{1/3} < 1.0,$$

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† The average atomic weight of a compound X_nY_m is simply $\bar{A} = (nA_x + mA_y)/(n+m)$, where A_x and A_y are the atomic weights of its constituents X and Y. The quantity Ω is then the average volume per kmol in the structure.

where N_0 is Avogadro's number (6.023×10^{26} kmol^{-1}) and the constant C depends on the packing: for FCC close-packing, for instance, it is 0.71; for open structures it can be as high as 1.0. We write this as the dimensionless group:

$$0.89 < b\left(\frac{N_0}{V_\mathrm{m}}\right)^{1/3} < 1.0. \tag{A 1}$$

(*b*) *The elastic moduli E, G, K and ν*

Young's modulus, E (GPa), the shear modulus, G (GPa), the bulk modulus, K (GPa) and Poisson's ratio (the negative ratio of lateral contraction to extension), ν (dimensionless) are related, for isotropic solids, by

$$G = \frac{E}{2(1+\nu)}$$

and

$$K = \frac{E}{3(1-2\nu)}.$$

For anisotropic solids these expressions are no longer exact, but can still be used as the basis of a dimensionless group. Poisson's ratio, for fundamental reasons, is constrained to lie in the range

$$-1 < \nu < \tfrac{1}{2}.$$

Foams and a few idiosyncratic solids can have values of ν anywhere in this range. For most materials, however, the ranges for ν are much narrower, generally in the range 0.2–0.4. Using these allows us to write limits for two simple groups:

$$C_\mathrm{L} < G/E < C_\mathrm{H} \tag{A 2}$$

and

$$C_\mathrm{L} < K/E < C_\mathrm{H}. \tag{A 3}$$

Typical values for C_L and C_H are listed in table 4.

(*c*) *Modulus E, melting point, T_m, and atomic volume, Ω*

If atomic bonds are stretched too far, they break. Heat, too, can break bonds, causing melting or sublimation. This is the basis of a relationship between elastic modulus and melting point. Bond stretching is characterized by the bulk modulus, K. Bonds fail at a strain of about 0.1, that is, at an extension of about $0.1b$, where b is the bond length, which we equate to the atom size. The work done in stretching one bond to failure is then $0.05Kb^3$ atom^{-1} or $0.05KV_\mathrm{m}$ kmol^{-1}. The thermal energy per atom or molecule at the melting point, T_m, is RT_m kmol^{-1} for each principal vibration mode (R, the gas constant, is 8.314 kJ kmol^{-1} K^{-1}). Equating these two gives

$$\tfrac{1}{200}KV_\mathrm{m} \approx RT_\mathrm{m}$$

or

$$C_\mathrm{L} < \frac{KV_\mathrm{m}}{RT_\mathrm{m}} < C_\mathrm{H}. \tag{A 4}$$

The constants C_L and C_H have the values shown in table 4. Note that the constants are of the order of 150, in surprisingly good agreement with the crude model outlined above. Young's modulus, E, is related to the bulk modulus, K (equation (A 3)), giving the associated correlation:

$$C_{\mathrm{L}} < \frac{EV_{\mathrm{m}}}{RT_{\mathrm{m}}} < C_{\mathrm{H}}. \tag{A 5}$$

For crystals and glasses and the constants have the same values as those of (A 4); but for elastomers and the more flexible polymers $E \ll K$ giving the smaller values of the constants shown for these solids in table 4.

(*d*) *Heat capacity, C_{p}, bulk modulus, K, melting point, T_{m}, and density, ρ*

The heat capacity is the heat required to raise the temperature of a solid by 1 K. Expressed as a molar heat capacity, $C_{\mathrm{v}}^{\mathrm{m}}$ (J kmol^{-1} K^{-1}),

$$C_{\mathrm{v}}^{\mathrm{m}} \approx 3R,$$

where R, as before, is the gas constant. If the (average) volume per kmol is V_{m} and the density of the solid is ρ, then the heat capacity, C_{v}, in the more usual units of J kg^{-1} K^{-1} is

$$C_{\mathrm{v}} = \frac{3R}{\rho V_{\mathrm{m}}}.$$

In the solid state, the heat capacity at constant pressure, C_{p}, is almost equal to that at constant volume, C_{v}, giving the correlation

$$C_{\mathrm{L}} < \frac{C_{\mathrm{p}}\rho V_{\mathrm{m}}}{R} < C_{\mathrm{H}}. \tag{A 6}$$

For most materials, C_{L} and C_{H} have values close to three. Materials with very high melting points, like diamond, are exceptional in that their Debye temperature lies above room temperature; for them C_{L} is lower.

Both equations (A 4) and (A 6) contain the quantity V_{m}/R. Eliminating it between the two gives the particulartly good correlation

$$C_{\mathrm{L}} < \frac{C_{\mathrm{p}}\rho T_{\mathrm{m}}}{K} < C_{\mathrm{H}}. \tag{A 7}$$

(*e*) *Expansion coefficient, α, bulk modulus, K, heat capactiy, C_{p}, density, ρ, and melting point, T_{m}*

The expansion coefficient, α, has its origins in the anharmonicity (asymmetric shape) of the force–distance curve which describes the atomic bonds. Gruneisen's model, based on the simplest sort of asymmetry, leads to the relationship

$$\alpha = \frac{\gamma_{\mathrm{G}}\rho C_{\mathrm{p}}}{K},$$

where γ_{G}, Gruneisen's constant, is a measure of this asymmetry: no asymmetry ($\gamma_{\mathrm{G}} = 0$), no expansion ($\alpha = 0$). Typically, $\gamma_{\mathrm{G}} \approx 1$ giving the correlation

$$C_{\mathrm{L}} < \frac{K\alpha}{\rho C_{\mathrm{p}}} < C_{\mathrm{H}}. \tag{A 8}$$

If this group is multiplied by that of equation (A 7) we obtain the particularly simple and useful correlation which was used as an example in § 3 *a*:

$$C_{\mathrm{L}} < \alpha T_{\mathrm{m}} < C_{\mathrm{H}}. \tag{A 9}$$

(*f*) *Thermal conductivity, λ, heat capacity, C_p, modulus, E, and electrical conductivity, σ_elec*

Heat transfer in non-metals is by phonons (lattice vibrations). Phonons are scattered by the lattice, by defects and by impurities and foreign atoms; their mean-free path between scattering events is nb, where b is the atom size and n is a number between one (highly disordered structures) and 100 (highly ordered structures). The theory of heat transfer by phonons then gives the thermal conductivity, λ ($\mathrm{W\,m^{-1}\,K^{-1}}$) as

$$\lambda = \tfrac{1}{3} nb\rho C_\mathrm{p} v,$$

where ρC_p is the heat capacity per unit volume ($\mathrm{J\,m^{-3}\,K^{-1}}$) and v is the velocity of sound in the material. Replacing v by $\sqrt{E/\rho}$ gives the correlation for non-metals:

$$C_\mathrm{L} < \frac{\lambda}{bC_\mathrm{p}\sqrt{E\rho}} < C_\mathrm{H}, \qquad \text{(A 10)}$$

with b given by $(\Omega/N_0)^{1/2}$ with $N_0 = 6.023 \times 10^{26}\ \mathrm{kmol^{-1}}$. The number n has been absorbed into the constants C_L and C_H with the consequence that values near the lower limit (C_L) are to be associated with disordered structures and those near the higher one (C_H) with highly ordered structures.

Heat transfer in metals has an additional large contribution from electrons, which travel much faster than phonons. The conductivity is given by an equation with the same form as that for phonons, but with C_p replaced by the thermal capacity of electrons, and v and nb by their velocity and mean-free path. Exactly these quantities appear in the expression for the electrical conductivity, σ_elec, of an electron conductor (a metal) leading to the Weidemann–Franz rule linking the two. In dimensionless form

$$C_\mathrm{L} < \frac{L\lambda e^2}{T\sigma_\mathrm{elec}k^2} < C_\mathrm{H}. \qquad \text{(A 11)}$$

The quantity L is the Lorenz number: $2.45 \times 10^{-8}\ \mathrm{V\,K^{-1}}$, e is the charge on an electron, T is the temperature and k is Boltzmann's constant.

(*g*) *Thermal diffusivity, α, thermal conductivity, λ, density, ρ, and specific heat, C_p*

The thermal diffusivity, α, is sometimes easier to measure than the conductivity, λ. They are approximately related by

$$a = \frac{\lambda}{\rho C_\mathrm{p}}.$$

When α and λ are measured independently, they are related (allowing for some experimental error) by

$$C_\mathrm{L} < \frac{a}{\rho C_\mathrm{p}\lambda} < C_\mathrm{H}, \qquad \text{(A 12)}$$

with C_L and C_H close to unity.

(*h*) *Latent heats of melting, L_m, bulk modulus, K, and melting point, T_m*

When a solid is heated, it melts, absorbing latent heat L_m. This is related to the thermal energy, RT_m, at the melting point. Expressing both in units of $\mathrm{J\,kmol^{-1}}$ (superscript 'm') gives 'Richard's rule':

$$C_\mathrm{L} < \frac{L_\mathrm{m}^\mathrm{m}}{RT_\mathrm{m}} < C_\mathrm{H}.$$

Re-expressing the latent heat in the more usual units of kJ kg^{-1} (symbol L_{m}) gives instead:

$$C_{\mathrm{L}} < \frac{L_{\mathrm{m}}\rho V_{\mathrm{m}}}{RT_{\mathrm{m}}} < C_{\mathrm{H}}. \tag{A 13}$$

Dividing this by equation (A 6) leads to

$$C_{\mathrm{L}} < \frac{L_{\mathrm{m}}}{C_{\mathrm{p}}T_{\mathrm{m}}} < C_{\mathrm{H}}. \tag{A 14}$$

Moduli are related to melting points by equation (A 4) giving

$$C_{\mathrm{L}} < \frac{L_{\mathrm{m}}\rho}{K} < C_{\mathrm{H}}. \tag{A 15}$$

Latent heats are helpful in the estimation of other properties, notably surface energies and various energies of formation and activation for point defects, though these are not discussed here.

(*i*) *Melting point, T_{m}, and glass temperature, T_{g}*

Some polymers crystallize to some extent and metallic glasses all crystallize if given the chance. For these the glass temperature T_{g} (K) and the melting point T_{m} (K) are empirically related (Beaman 1952) by

$$0.5 < T_{\mathrm{g}}/T_{\mathrm{m}} < 0.75. \tag{A 16}$$

(*j*) *Relationships between measures of strength (σ_{y}, σ_{c}, σ_{ts}, σ_{MOR}, σ_{e}, σ_{f} and H) and stiffness (E, K and G)*

The elastic limit, σ_{y} (MPa), of ductile solids is the stress at which dislocations first move large distances. It correlates loosely with the modulus E (in MPa) because dislocation line tensions and interaction energies scale as E, but the range C_{L} to C_{H} is wide. Metals with non-local bonding such as copper can deform plastically at stresses as low as $E/10^5$. For polymers the correlation is better (they deform at about $E/50$). Thus we may write

$$C_{\mathrm{L}} < \sigma_{\mathrm{y}}/E < C_{\mathrm{H}}. \tag{A 17}$$

Materials with highly localized bonding such as ceramics and inorganic glasses deform plastically only at stresses of the order $E/20$. They generally fracture before dislocation plasticity starts, so their elastic limit and fracture strength, σ_{f}, are the same as their tensile strength, σ_{ts}. Ductile solids yield before they fracture; for these the tensile strength and fracture strength are greater than the elastic limit by a factor of between 1.1 and 5. Thus we may write

$$C_{\mathrm{L}} < \sigma_{\mathrm{ts}}/\sigma_{\mathrm{y}} < C_{\mathrm{H}}, \tag{A 18}$$

in which we identify σ_{ts} with the fracture strength σ_{f} for brittle solids. Combining this with (A 17) gives

$$C_{\mathrm{L}} < \sigma_{\mathrm{ts}}/E < C_{\mathrm{H}}. \tag{A 19}$$

The modulus of rupture σ_{MOR} (MPa) is the maximum surface stress at which failure occurs in a beam loaded in bending. It is generally rather larger than the fracture strength in tension σ_{f} (MPa), giving

$$C_{\mathrm{L}} < \sigma_{\mathrm{MOR}}/\sigma_{\mathrm{f}} < C_{\mathrm{H}}. \tag{A 20}$$

The compressed strength, σ_c (MPa) for metals, is almost exactly the same as that in tension, σ_y (MPa). For other classes of solid the two differ by a factor on which limits can be placed. The relationship is described by

$$C_L < \sigma_c/\sigma_y < C_H. \tag{A 21}$$

The hardness is often given as a Vickers number, H_V. The hardness, H (MPa), is related to this by $H = 10H_V$, and to the yield stength σ_y (MPa), for soft plastic materials, by

$$C_L < H/\sigma_y < C_H. \tag{A 22}$$

If σ_y is interpreted as the yield strength at a strain 8% larger than at first contact, the constants have the values $C_L = 2.6$ and $C_H = 5$. For harder materials, when σ_y becomes large, elastic spring-back increases the perceived hardness leading to larger values of C_L and C_H.

Finally, the endurance limit in fatigue, σ_e (MPa), is related to the tensile strength, σ_{ts} (MPa), by the 'fatigue ratio':

$$C_L < \sigma_e/\sigma_{ts} < C_H, \tag{A 23}$$

with C_L and C_H in the range 0.5–0.95.

(*k*) *Relationships between measures of toughness (K_{Ic}, G_c and ΔK_{TH}) and of strength (σ_y) and stiffness (E)*

The fracture toughness K_{Ic} (MPa m$^{1/2}$) is related to the yield strength, σ_y (MPa), and the atom size, b (m), by

$$C_L < \frac{K_{Ic}}{\sigma_y\sqrt{b}} < C_H. \tag{A 24}$$

and to the modulus, E (MPa), by

$$C_L < \frac{K_{Ic}}{E\sqrt{b}} < C_H. \tag{A 25}$$

Since G_{Ic} is related to K_{Ic} by $EG_{Ic} \approx K_{Ic}^2$ we find

$$C_L < G_{Ic}/Eb < C_H. \tag{A 26}$$

A lower limit for G_{Ic} is 2γ where γ is the surface energy of the solid. Since the surface energy of solids is roughly $Eb/20$, we find a lower limit for C_L of 0.1.

(*l*) *Other correlations*

There are many more such correlations (Beaman 1952; Davies 1976; Brown & Ashby 1980*a*, *b*; Frost & Ashby 1982; Sammis *et al.* 1981; Fisher 1988). They relate surface properties to bulk properties; they describe kinetic constants such as activation energies, and they relate the temperature and pressure dependences of properties to the melting points and bulk moduli. To keep this paper manageable, they will not be listed here. Their existence suggests that the method can be extended further.

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