PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Technology of the 1990s: Advanced Materials and Predictive Design [and Discussion]

M. F. Ashby, S. F. Bush, N. Swindells, R. Bullough, G. Ellison, Y. Lindblom, R. W. Cahn and J. F. Barnes

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Technology of the 1990s: advanced materials and predictive design

By M. F. Ashby, F.R.S.

Cambridge University Engineering Department, Trumpington Street, Cambridge CB2 1PZ, U.K.

The demands made on materials in contemporary design are increasingly stringent. Materials and design methods have evolved to meet them. However, it is proving increasingly difficult to extend current design methods, largely based on continuum modelling and empiricism, to cope with the larger number of variables that appear in many engineering applications. It is argued that atomistic modelling (which, by itself, seldom leads to engineering solutions) can give additional insight into the form of constitutive equations, the grouping of variables, and the magnitudes of material properties. Properly interpreted, this information can point the way to a 'model-informed' empiricism that can help solve pressing engineering problems.

1. The evolution of materials

This symposium seeks an overview of the materials in the 1990s; a perspective on where materials are going. Historians tell you that, to look forward, it is often helpful first to look back. A perspective requires a long view.

Before 2000 B.C. cutting tools were mostly made of flint. Flint is a ceramic, and was an important material in an age when stone, pottery and wood were almost the only engineering materials. Metals were unknown. Flint had a special role, because it could be shaped to a cutting edge and used as a weapon or as a knife. It was one of the engineering materials of the stone age, or – as we would now call it – the age of ceramics (figure 1). It was an era in which metals played almost no role; engineering (housing, boats, weapons, utensils) was dominated by polymers (wood, straw, skins), composites (like straw bricks) and ceramics (stone, pottery and, later, glass).

There was a time when the standard of living of a country or community could, presumably, be measured by the flint consumption per head of population. However, as ways were discovered to make metals, they began to displace ceramics. Around 1500 B.C. the consumption of bronze probably revealed who were the world powers; and still later, iron. Since 1850 it has been steel: economists correlate the level of development of a country with the quantity of steel it produces per head of population. From this point on, metals dominated engineering design. Their position was strengthened by the development of the alloy steels, the light alloys (replacing wood in aircraft design) and the superalloys. By 1960 'materials' was synonimous with 'metallurgy'; the world's universities taught courses and awarded degrees in metallurgy and metal science; the graduates had barely heard of polymers, ceramics and composites.

However, in the past 20 years that has changed. The steel industry, world wide, is declining, and the rate of development of other metals and alloys appears to have slowed. The production of other classes of materials – high-strength polymers, ceramics, structural composites – is expanding, or is poised to do so (figure 1). The production of carbon-fibre based composites, for instance, is growing at about 30% per year; that is the sort of growth rate enjoyed by steel

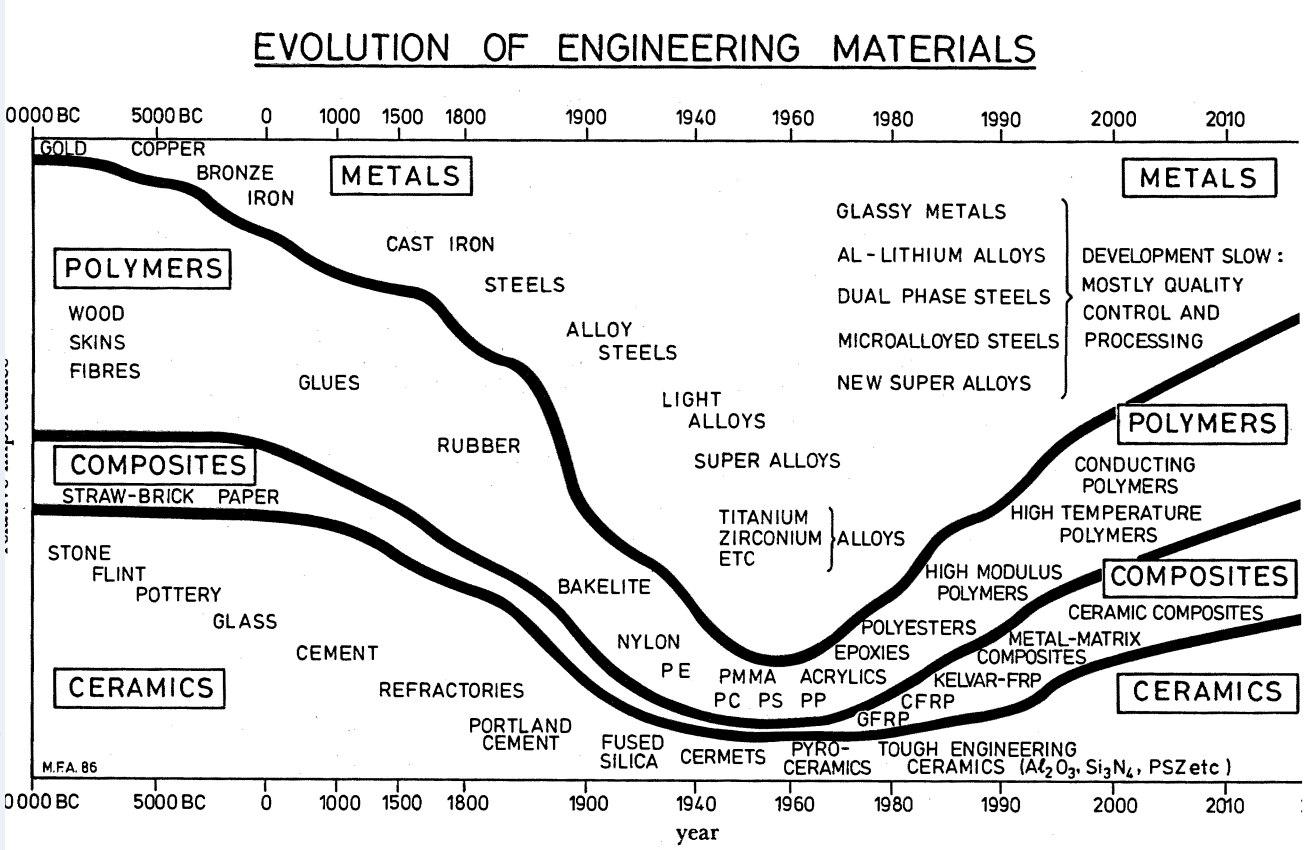

FIGURE 1. The evolution of materials for mechanical and civil engineering. The relative importance of four classes of materials (polymers, composites and ceramics) is shown as a function of time. The diagram is, of course, schematic, and does not describe either tonnage or value. The timescale is nonlinear.

and the peak of the industrial revolution. We are just now in the middle of another revolution, a transition from the steel age to one dependent on other, more advanced, materials. Such changes tend to be discontinuous and rapid, and the disruption caused by the change creates social and economic problems. However, the new materials offer new and exciting possibilities for the designer: the potential for new products and the scope for major improvements in old ones.

Realizing this promise requires more than just the new material; very little is gained without innovation in design. Surveying the history of design is less easy, but it is instructive to try.

2. DESIGN WITH MATERIALS

Early mechanical design was empirical. You tried it, and if it worked you used that method again. If it fell down, you tried something different. The store of empirical knowledge accumulated in this way is vast; it was the basis of almost all design until the middle of the last century, and much design, even today, uses it. It is one of the foundations of current practice (figure 2).

Modern mechanical design uses two other boxes of tools. The first I have called 'mathematics and continuum modelling'. Materials obey certain experimentally observed rules: the 'laws' of mechanics of thermodynamics, of rate theory, and so forth. From these have evolved the

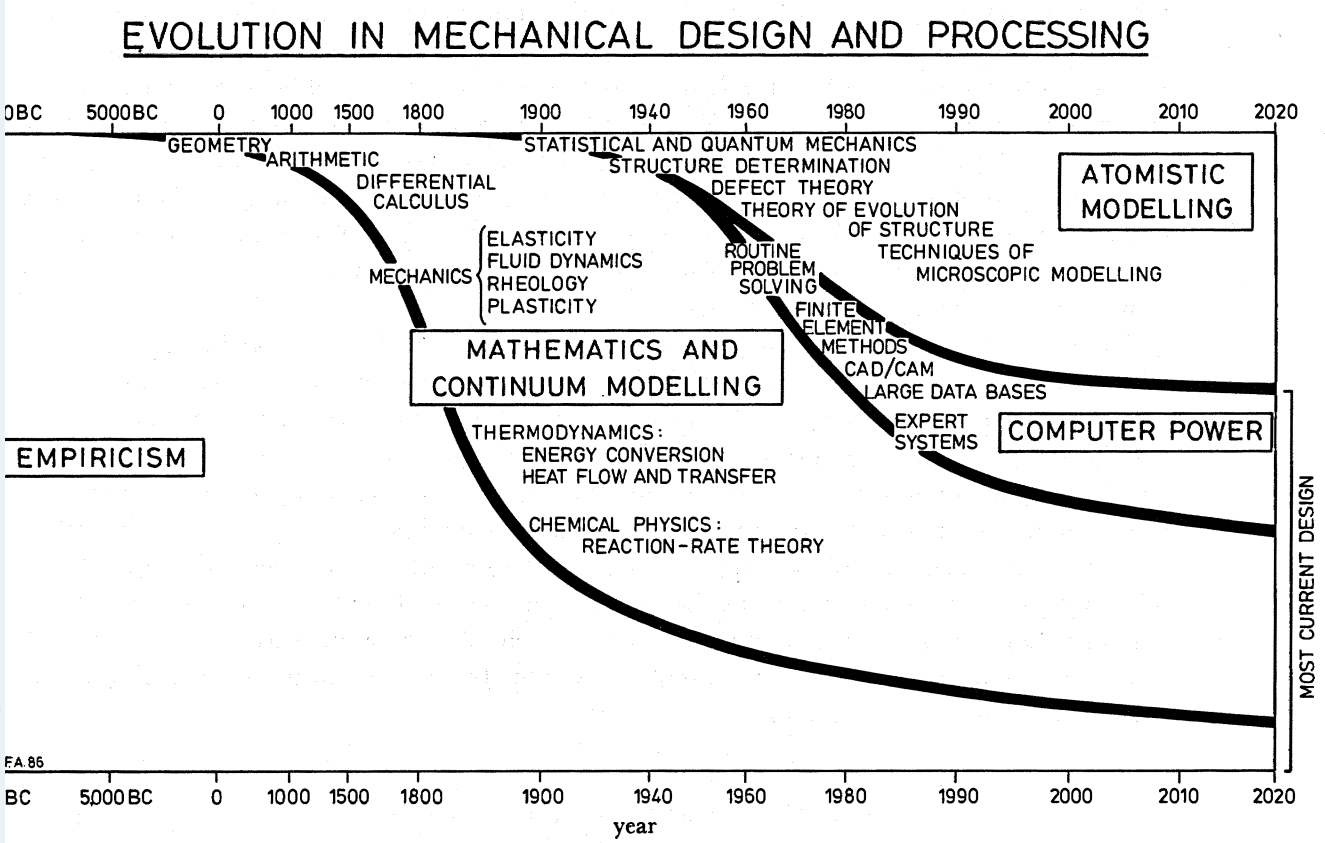

FIGURE 2. The evolution in mechanical design and processing. The relative importance of empiricism and of continuum modelling (aided by computer power) is shown, schematically, as a function of time. It is argued that atomistic modelling can contribute more than, at present, it does. The timescale is nonlinear.

continuum theories of elasticity, plasticity, fluid flow, heat flow, diffusion, and reaction rates. They can be thought of as a sort of 'distilled empiricism', which embodies, in a way that can be manipulated by mathematical methods, the simplified results of a vast amount of experimentation. Continuum design is a very powerful tool. However, it is important to realize its limitations. It provides a *description* of material response to certain stimuli (like tensile stress at room temperature). It gives no help, however, in *predicting* the response of a material to a new stimulus (like multiaxial stress at elevated temperature) because it contains no information about mechanisms: a description of the material response to a new stimulus requires a completely new set of experiments from which new continuum rules must be distilled. Also, the method gives no help in predicting the *magnitudes* of material properties. Young's modulus enters Hooke's law as a material property that must be measured; the law gives no indication of its value. However, continuum methods are still important: most modern mechanical design is based on them.

Their scope has been enormously extended by the recent development of computer power, which one might regard as the third of the three foundations of modern design (figure 2). Computer power is now so cheap that techniques that once were applied only to critical components can now be applied to all; and this permits an optimization to minimize cost, or to maximize performance or safety, which was not previously possible.

In parallel with all this, there have been other developments, which I will call 'atomistic

modelling' (figure 2). Over the past 100 years, the understanding of materials at the atomistic and electronic level has increased immensely. Diffraction of radiation and of particles has elucidated structure. Quantum mechanics has explained the nature of bonding and predicted the magnitude of properties such as Young's modulus. Statistical mechanics has provided the fundamental basis for reaction-rate theory, and allowed the modelling of structural change (the heat-treatment of steels, for example). Defect theory – particularly the theory of point defects, of dislocations and of crystal boundaries – now gives a detailed picture of the atomistic aspects of deformation, of creep and of fracture. However, all this has had remarkably little direct influence on design in mechanical engineering.†

There are good reasons for this. Atomistic models contain *microscopic parameters*: molecular vibration frequencies, mobile dislocation densities, interaction potentials between atoms, or local concentrations of impurity, which vary widely. In any real engineering material they are simply not known with useful precision. They can, of course, be measured – by probing the structure appropriately with X-rays, or by magnetic resonance, or by secondary-ion mass spectrometry – but it is not practical to apply these techniques to (let us say) the routine manufacture of piston rings. The engineer needs procedures that depend only on *macroscopically measurable properties*: you could check the hardness of every turbine blade (if you had to); you could not hope to measure its mobile dislocation density. So while the learned journals are full of atomistic models for creep (for example), these models are not used by the engineer who designs high-temperature equipment.

3. Materials selection in design

Consider the design of a simple mechanical component, such as a spring. Springs are devices for storing energy; they can be made out of almost anything. You can make a spring out of wood, for example; longbows were made of wood for generations. If you have generations in which to perfect them, you can try various shapes and lengths and profiles, and you can experiment with various sorts of wood, until, empirically, you have arrived at a pretty good design. It takes time, because there are many variables, and the number of experiments goes up steeply with the number of variables: three woods, three lengths and three thicknesses of bow requires 27 tests. Experience, it is true, helps reduce the number: if a short bow made of oak is no good, a short bow made of ash is not likely to be much better. The design of a bow, however, involves many more variables than this – profile, and the way it varies along the bow, for instance – so that the development programme, if purely empirical, is a long one.

That is where continuum modelling has revolutionized design. The bow must store as much energy as possible for a given pull-force and displacement. It must return this energy (and not dissipate it as heat) when released. Also it must be as light as possible so that the archer can carry it without fatigue. Those requirements can be recast in terms of beam theory: it is a question of optimizing the stiffness of a beam, subject to certain constraints. That is exactly what continuum mechanics is good at: the best length and thickness, and the best choice of material, can be calculated in a few moments without an elaborate test programme. If computing power is available, the same methods allow you to calculate the optimum profile of the bow as well.

† Design of electronic materials is different. Semiconducting devices are derived directly from the understanding of electrons in solids.

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So continuum design methods are very powerful. You still have to make and test bows, of course, but far fewer of them. If you examine more closely what has happened, it is that the continuum theory has *grouped* the variables. The first constraint – that the draw force be the strength of a man – reduces the number of independent variables by one; the second – that the draw displacement be the length of your arm – removes a second; each new constraint (minimum mass, for instance) removes another. If you are lucky, you end up with a single, dimensionless, group: the design is completely constrained. Even if you are not – if the design has some aspects that you cannot model accurately (like fatigue of the bow, or fretting where the string attaches to it) – the number of tests you have to do is vastly reduced. Empiricism always contributes; but its contribution is more to the fine-tuning than to the basic design. That, of course, is an over-simplification: it undervalues the vast store of empirical knowledge that a good designer brings to bear on the problem. However, the important point is that the continuum modelling reduces enormously the number of experiments you have to do, and guides you more efficiently to the optimum design.

However, as the conditions under which materials are used become more severe, and as the need for a higher level of optimization (for safety, economy, performance) grows, the continuum method begins to run out of steam. The problem is that the constitutive equations of continuum design are based on experiment. Hooke's law is a statement of an experimental observation: that strain is proportional to stress. So are the equations of heat flow and of fluid flow and of plasticity. Continuum theory is, as we have said, distilled empiricism, formulated in a way that makes it compatible with mathematical methods, and thus able to be generalized. Experiments on the draw force of a bow do not give much help in designing, let us say, a helical spring. But experiments designed to measure strain as a function of stress for a material, when coupled with simple statements of equilibrium and compatibility, allow both the bow and the helical spring to be designed (figure 3, top-left box).

The difficulty arises when conditions become more stringent, so that more properties are involved. A spring for use at high temperature may suffer from creep. The loads on it fluctuate, so it may fatigue. The environment may be unpleasant, so it may corrode. The stress state is not simple tension or bending and there may be mean stresses that are non-zero as well as oscillating stresses. We need constitutive equations for design that include all of these. The experimental programme to devise them become formidable: there are too many variables again. Worse, when mechanisms of failure *interact*, superposition becomes important; and if the interactions are nonlinear, the simple constitutive laws break down. And as mentioned earlier, the continuum approach says nothing about the magnitudes of material properties. So it gives no guidance in selecting between new materials, or in designing them.

This is where atomistic modelling can help (top row, figure 3). It seeks to identify atomistic processes responsible for creep, for fatigue, and for corrosion, and to use the understanding derived from the theory of bonding, of defects, of reaction rates (and so forth) to model them. The problem is that the models, although physically sound, are rarely precise enough to be of much use to an engineer. If your predicted creep rate (in this sort of modelling) is within a factor of ten of the observed rate, you are doing well. The method based on pure atomistic modelling breaks down in the precise knowledge of certain microscopic variables, like grain boundary diffusion rates, jump frequencies or mobile dislocation densities, that cannot easily be measured.

But the atomistic models give something else. They have certain broad features, which,

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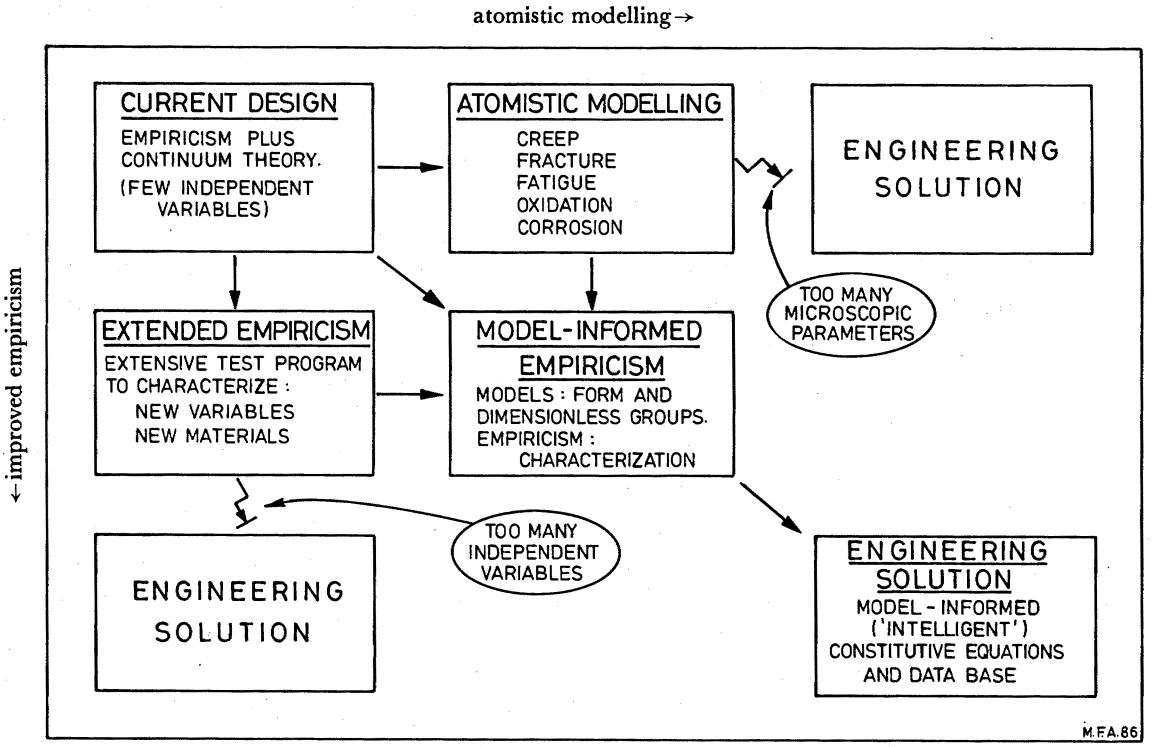

FIGURE 3. Three possible routes towards an engineering solution to a complex design problem involving materials. Starting from the top left, there is the route of improved empiricism, that of atomistic modelling, and the coupled route of model-informed empiricism. The last appears to be the most promising.

properly interpreted, point to rules that the constitutive equations must obey: rules which govern rules, so to speak; the computer scientist calls them 'metarules'. Some have been known and used for a long time. Both creep and oxidation are thermally activated processes, so models based on statistical mechanics lead us to expect a rate that depends on temperature as

$$\text{rate} \propto \exp(-Q/RT) \tag{1}$$

at least over the range of temperature for which one mechanism dominates. The matarules help us to group the variables in new ways, reducing the number which are independent (examples in a moment). And the atomistic theory of solids gives us information of a different kind. It suggests, for instance, that the activation energy, Q, should scale as the melting point, T_m (for a crystalline solid) or the glass temperature T_g (for an amorphous solid) so that

$$Q/RT_m = \text{const. (crystal)},$$
$$Q/RT_g = \text{const. (glass)}, \tag{2}$$

This allows the creep rate in one material to be inferred from that in another. Similar statements can be made about the effect of pressure, alloying, precipitation or radiation. The point is that, although atomistic models cannot, by themselves, lead to precise constitutive laws, they do suggest the form that the laws should take, and they put limits (often quite close limits) on the values of the physical constants (like Q) that enter them.

The way to exploit this is to follow the path of 'model-informed empiricism', illustrated by

the diagonal of figure 3. The models suggest forms for the constitutive equations, and for the significant groupings of the variables that enter them; empirical methods can then be used to establish the precise functional relations between these groups. The result is a constitutive equation that contains the predictive power of atomistic modelling with the precision of ordinary curve-fitting. In parallel, the broad rules governing material properties can be exploited to create and check the data base of material properties that enter the equations. You might think all this so obvious that it hardly needs saying, but its potential contribution to mechanical engineering is only just being recognized and dignified by the title of 'intelligent' design and processing (Wolf 1986). Two examples may help to illustrate this.

4. Example: design against creep

Consider first design against creep. Creep is slow deformation, which accumulates with time. It is a problem in high-temperature energy-conversion equipment, turbines, nuclear reactors, etc. (It is less familiar than other deformation mechanisms, because most metals do not creep at room temperature. Creep only becomes a serious problem at temperatures of more than one third of the melting point. So steel does not creep below about 300 °C. Computing the extent of this sort of deformation is difficult because it depends in a sensitive way on both stress and temperature, and these, it should be remembered, are not constant; in any real turbine or reactor they vary with time. The goal of creep design is to predict the creep strain, and any consequences of it, like fracture. With increasing emphasis on efficiency and on safety, the premium on precise creep prediction is great

Current methods of design against creep are empirical (figure 4, top-left box). The strain–time curve is approximated as a straight line, with a slope which depends on two independent variables: stress, σ, and temperature, T. With only two such variables, a fairly complete characterization is practicable. The result, for a limited range of the variables, is often written:

$$\epsilon = A\sigma^n[\exp-(Q/RT)]\,t, \tag{3}$$

where ϵ is the creep strain that has appeared in time t, n is a constant exponent, and A and Q are constants. The equation is used to predict creep strain, and as a basis for extrapolation, life prediction and other such design calculations. But the equation does not include primary or tertiary creep, nor does it cater for time-varying stress and temperature, or for the effect of stress-state on creep fracture. If we try to include them, we find we are dealing with eight or more independent variables: temperature, stress, the frequency (ν_T, ν_σ) and amplitude (ΔT, $\Delta\sigma$) or both, the ratios λ of stress invariants and so on:

$$\epsilon = f(\sigma, \lambda, T, t, \Delta\sigma, \Delta T, \nu_\sigma, \nu_T, \text{etc.}) \tag{4}$$

It is possible to set up an experimental programme to characterize the influence of each of these variables on creep; that is the direction in which research has moved (downwards on figure 4). However, the scope of the test programme is immense; and it is sometimes found that more than one *mechanism* of creep and of fracture may be involved, and that the characterization of one range of temperature (for instance) cannot safely be extrapolated into another; a new characterization is needed. The method of extended empiricism breaks down under the load of variables.

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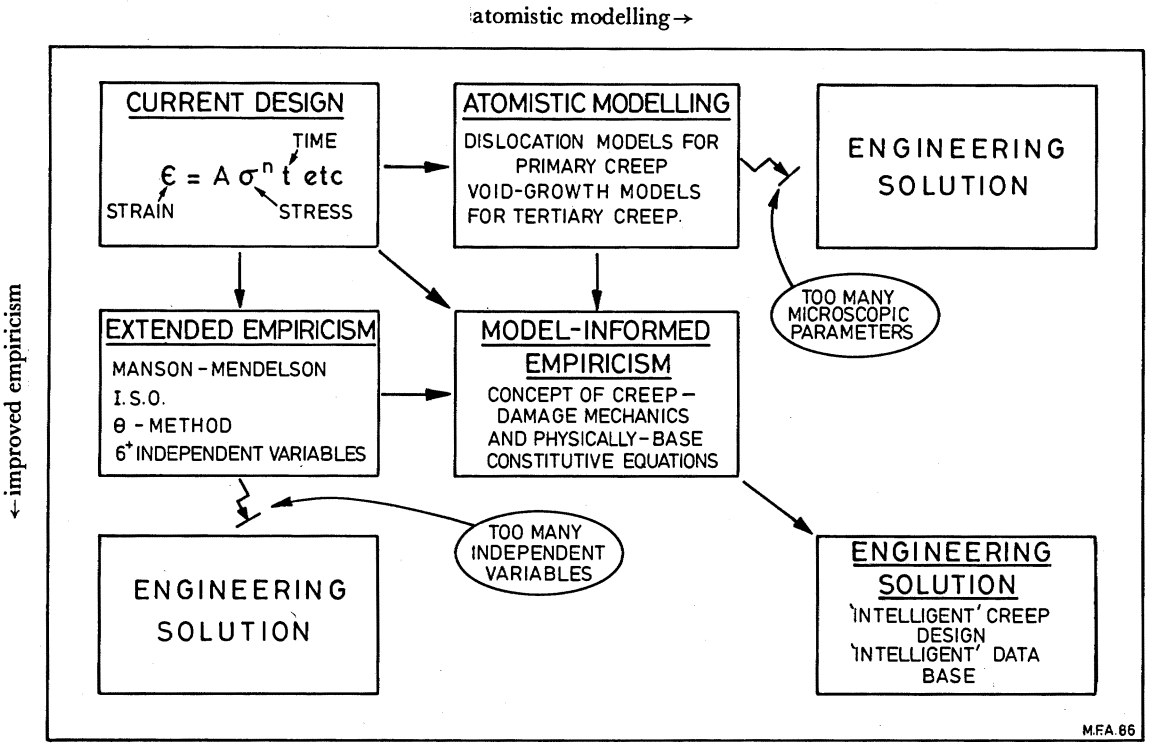

FIGURE 4. Design against creep. Extending the current empiricism (first column) is difficult because there are too many variables. Developing atomistic models (top row) results in equations with too many microscopic parameters. Combining ideas from both paths leads to the concept of 'damage mechanics' (diagonal), which offers new potential for design against creep.

Atomistic modelling follows a different path (figure 4, top row). It seeks to identify the underlying atomistic processes responsible for creep: viscous flow, diffusion, time-dependent dislocation motion, grain-boundary sliding, void growth and so forth and to model each stage of creep from first principles. It has had some success: the mechanisms giving creep and creep fracture are now tolerably well understood although not, in engineering terms, well characterized. The problem (as I have already said) arises because the atomistic models contain microscopic parameters: the density of obstacles to dislocation motion, the density of void nuclei, etc., which can only be determined by microscopic measurement, and this, in an engineering context, is not practical.

However, the models point to something else, and it is of the greatest value; they suggest the proper form that the constitutive equation should take. All models for primary and steady creep have in common that they lead to equations not for strain, but for *strain rate*, and that they contain an *internal state variable*: a parameter that characterizes the current mechanical state of the material. Models for tertiary creep and fracture have the same feature: they lead to equations for *rates* and they contain an internal state variable (often the area fraction of cracks or voids) which evolves during creep (Ashby & Dyson 1985; Ion *et al.* 1986). We will call these internal variables 'damage' because they describe a change in the state of a material, brought about by creep. The models suggest a constitutive equation with a completely different form than before. Instead of trying to characterize strain, ϵ, as a function of the independent

variables, we now seek to fit data to a coupled set of differential equations, one for strain rate, $\dot{\epsilon}$, and two more for damage evolution, $\dot{D}_1$ and $\dot{D}_2$:

$$\left.\begin{aligned}\dot{\epsilon} &= g(\sigma, T, \lambda, D_1, D_2),\\ \dot{D}_1 &= h_1(\sigma, T, \lambda, D_1, D_2),\\ \dot{D}_2 &= h_2(\sigma, T, \lambda, D_1, D_2),\end{aligned}\right\} \tag{5}$$

where D_1 describes the primary creep damage and D_2 describes the tertiary damage leading to fracture and $\dot{D}_1$ and $\dot{D}_2$ are their rates of change with time; g, h_1 and h_2 are simple functions. At first sight, this may seem to have complicated the problem. However, there are only three independent variables (σ, T and stress state, λ) whereas before there were eight. Also, the individual equations are simpler than before, and (more important) they include, in a physically sensible way, the ability to cope with arbitrarily varying stress and temperature. With modest computer power, the equations can be integrated to track out the evolution of strain and damage, and ultimately, to predict fracture in a component. Equation (5) can now be adopted as the constitutive equation for creep, and empirical methods can be used to determine the functions g, h_1 and h_2. This 'model-informed empiricism' (diagonal on figure 4) has lead to the development of a new branch of mechanics (generally called damage mechanics), which has applications far beyond the narrow field of creep.

5. Example: controlling the heat-affected zone of welds

Consider a second example, one in the area of processing and fabrication. Most material processing is empirically based. Even welding, a relatively sophisticated and critical operation, is carried out by methods that rely largely on direct experiment. The results of these experiments are summarized in tables and charts from which the welding conditions appropriate for a given job are chosen. The method is, of course, informed by an enormous body of metallurgical knowledge and experience; but the contribution of atomistic modelling is negligible.

A concern with welds is the condition of the heat-affected zone (HAZ); it is the region on either side of the weld itself. Within this zone the structure of the parent plate has been altered by the heat conducted into it from the weld. This heat cycle is not sufficient to melt the zone, but it is enough to cause precipitates to coarsen or dissolve (given weakness in aluminium alloys) and to cause grains to grow (with risk of martensite, and thus of cracking, in steels). Failures in welds often start in the HAZ.

Current welding practice, embodied in the tables and charts that I have mentioned, gives warning of this problem, and advises of the welding conditions that will cause it. But the data on which the charts are based comes from a limited range of experimental conditions. It is difficult to do better than this because the number of variables is large, and because it is difficult to extrapolate the data that *is* available to other more extreme conditions, because the underlying processes are complex and nonlinear.

Look first at the number of variables (first column, figure 5). When a weld torch tracks across a metal plate, the temperature at a point in the plate rises and then falls again. The shape of the cycle depends on six *thermal variables*; the torch power, q, its tracking speed, v, the diameter of the flame or arc, $2r$, the thickness of the plate, t, its thermal conductivity, λ, and specific heat, c. What the heat cycle does to the plate depends on a further set of *metallurgical variables*:

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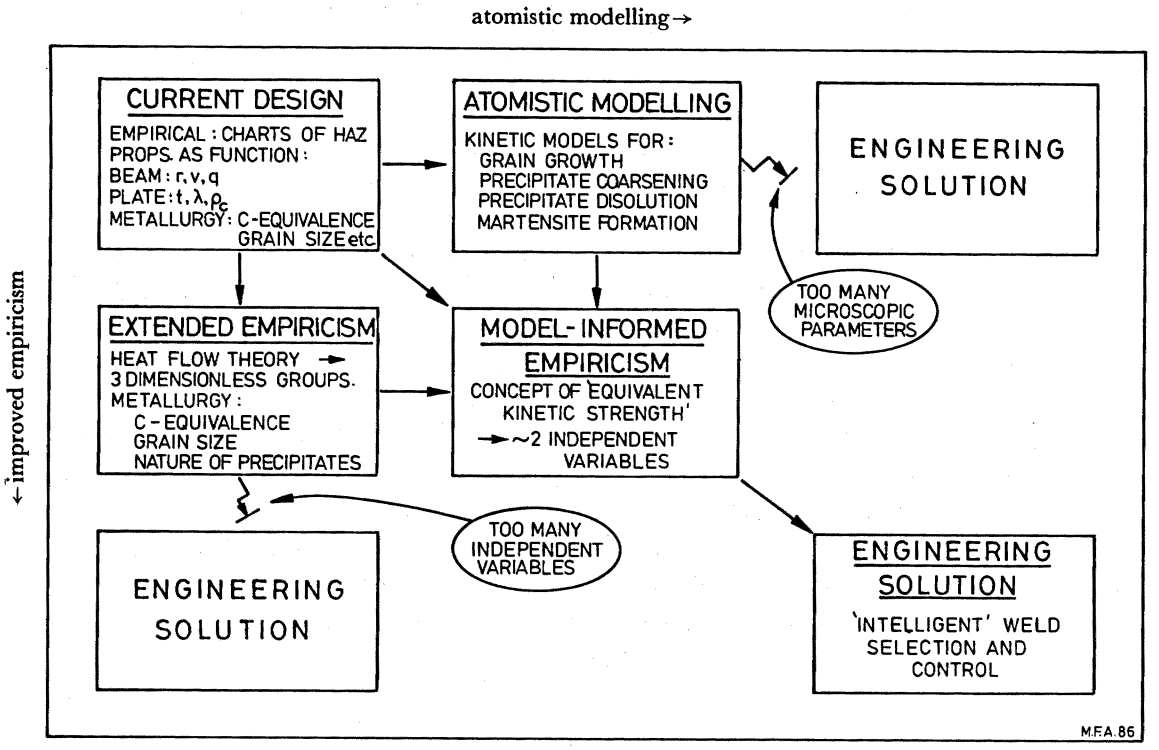

FIGURE 5. Process modelling and control. The width and properties of the heat-affected zone (HAZ) of a weld depend on process variables like beam energy, q, radius, r, and velocity, v, and on the thickness, t, of the plate being welded, and the thermal and metallurgical properties of the plate. Extended empiricism is made difficult by the large number of these variables. Atomistic models suggest a way of combining them in the 'equivalent kinetic strength' of the weld cycle, which greatly reduces the number of variables.

the grain size, the alloy concentration, the state of ageing or precipitation, and so forth: even in the simplest alloy there are at least two such variables, usually many more.

A full empirical characterization of a problem with eight independent variables is a daunting business. But here the theory of heat flow (Carslaw & Jaeger 1959) can help. It tells us that the variables of heat flow can be grouped into three dimensionless groups; the temperature at any point below the surface depends only on these. There are only three independent variables, not six, associated with calculating the temperature in the heat-affected zone. No atomistics are involved here; this is merely an application of the continuum theory of heat flow. However, even with this simplification, the number of variables is still large.

The metallurgical changes are more difficult. This is where atomistic modelling can contribute (Ashby & Easterling 1982; Ion *et al.* 1984) (top row of figure 5). Models for grain growth, for precipitate coarsening, for precipitate dissolution, and so forth, are well developed. However, like those for creep, they contain microscopic parameters (kinetic constants, interface diffusion coefficients and so on), the magnitudes of which are not known with precision. All the models, however, have the common feature that the rate of change of the property (which we shall call ϕ: it might, for instance, be the grain size) is related to its current value, and to the instantaneous temperature $T(t)$ by:

$$\mathrm{d}\phi/\mathrm{d}t = f(\phi)\,\exp -\{Q/RT(t)\}, \tag{6}$$

where $f(\phi)$ is some (often complicated) function of ϕ. The total change in this property during a weld cycle at some point within the heat-affected zone, is then given by:

$$\int_{\phi_1}^{\phi_2} \frac{\mathrm{d}\phi}{f(\phi)} = \int_0^{\infty} \exp - \left\{\frac{Q}{RT(t)}\right\} \mathrm{d}t. \tag{7}$$

A given change in the property means a given, constant, value for the left-hand side of the equation, and thus for the right-hand side also. So the integral on the right-hand side determines the extent of the structural change. It can be thought of as *the equivalent kinetic strength* of the weld cycle; it measures the number of kinetic jumps that occur during the cycle (central box of figure 5). For a given weld cycle, $T(t)$ is known and the integral can be evaluated. The particulars of the structural change are contained in the quantity Q, which is the characteristic activation energy for this change. This reduces the number of variables characterizing the change to one: any weld process with a given value of equivalent kinetic strength, S, produces the same degree of structural change. This is an immense simplification and holds the potential for the considerable rationalization of these (and other) types of processing.

6. Conclusions

The demands made on materials in modern design are increasingly stringent. Higher performance, greater economy, increased reliability and safety all require that the designer knows more about the materials he uses. This knowledge is partly contained in the constitutive equations of continuum design, and in the form of empirical knowledge and experience. Extending it is proving difficult because the number of service or process variable required for sophisticated, optimal, design is large.

Atomistic models for processing and for service performance have, until now, had little impact on mechanical design. It is because they are too firmly rooted in the underlying atomistic processes which, though understood, can be characterized only by microscopic measurements, which are impractical for the engineer.

One way forward is to seek to identify the broad rules governing material behaviour, and the rules governing the magnitudes of material properties, which are contained in the atomistic models, and use these as the basis of a 'model-informed' empiricism. There is, of course, precedent for this: much 'empirical' design has, buried in it, concepts borrowed from solid-state theory. However, even a quick look at two important areas, design against creep and process-control in welding shows that the potential gains have not been fully exploited. They are considerable.

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Discussion

S. F. Bush (*University of Manchester, Institute of Science and Technology, U.K.*). The concept described is a welcome alternative to trying to model the details of every particular situation. The polymer flow field offers similar incentives and opportunity. Manufacturers' data for flow, essentially viscosity, is provided at a particular temperature, and at a particular strain-rate only. Such data do not allow one to predict flow behaviour in a real case, moulding for instance, because both temperature and strain rate vary considerably from point to point. An alternative to trying to provide viscosity data for each point is to decompose the pseudoproperty viscosity into a few variables that reflect directly the molecular chain structure of the material, however crudely. From this step, two or three more fundamental (i.e. molecular) variables or variable groups are deducible, which generate the flow behaviour directly, largely bypassing viscosity as a property of the material, seeing it rather as an outcome of the flow process.

The approach seems to parallel very closely the procedures described by Professor Ashby for creep where the variables D_1, D_2 are introduced to mirror key aspects of the creep process at an atomistic level in such a way as to have broad, if approximate application, across a wider range of materials and conditions than purely curve-fit relations for creep can do.

M. F. Ashby. I find Professor Bush's comment most interesting. There is clearly scope for unification of the approach to describing viscosity which Professor Bush mentions, and the damage-mechanics approach which is widely used to describe creep.

N. Swindells (*Matsel Systems Ltd, Liverpool, U.K.*). The modelling techniques described by Professor Ashby have an important connection with the requirements for computerized materials information systems discussed in the previous paper by Dr Westbrook. Materials information systems can be considered in two groups: data systems, which would contain the results of tests or other sources of measured values, and knowledge systems, which would add value to collections of results by dealing with the relations between measured values. Knowledge systems would therefore either encapsulate existing understanding or enable new knowledge to be created and such systems are in active development.

Data systems will not usually be complete because of the origins of their information but if knowledge systems are to be useful they must be complete. The important role for models therefore lies in extending knowledge into areas where there is no, or inadequate data and, given the view that in knowledge systems, the information can be at a lower level of precision, the models would enable knowledge systems to become more complete.

M. F. Ashby. I agree with Professor Swindells's comments. Knowledge-based systems are best constructed around models of material behaviour. There is, I believe, great scope for the development of modelling as a component of intelligent processing and intelligent materials selection.

R. Bullough, F.R.S. (*AERE, Oxfordshire, U.K.*). I very much enjoyed Professor Ashby's contribution and, as exemplified by my own work on the theory of radiation damage in metals, I very much agree that any data field is best described with the aid of a physically based model or set of models. The data set can then be used to determine any unknown parameters in such

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models and one can thereby confidently extrapolate beyond the data base with due recognition of any mechanism change that might occur. However, I was interested in the distinction he drew between continuum and atomic models and reference was made to the existences of a 'bridge' between the two. I wonder what his view is of the various generalized continuum approaches such as 'non-local' and 'director' continua; the latter was used to describe the 'continuously dislocated crystalline media' when each point of the continuum has a triad of vectors that describe the local crystallinity and the former enables the tools of integro–differential calculus to be used to describe long-range interatomic forces and dispersive effects, etc.

Whereas I personally doubt very much whether the various non-local continua are really helpful in creating a bridge I would like to think that someday the concept of the continuously dislocated crystal might help to bridge the gap between the classical plasticity approach and the use of discrete dislocation (or atomic) models. In principle when the response of a body depends on the collective motion of dislocations and other crystalline defects, such a distribution approach might be useful; however, when the response is a highly localized event, like fracture, it is clearly inappropriate

M. F. Ashby. The concept of the continuously dislocated crystal is a very appealing one. It has been around for some time, and has had success in describing the internal state of single crystals subjected to simple deformation modes such as pure bending or torsion. The difficulty, I think, is that of describing other deformation states (by pure shear, or simple tension) in which the first moment of the dislocation density (the spacial average) is zero. A second problem arises in attempting to calculate the strength of materials in which the obstacle spacing is comparable with that of the the dislocations themselves (dispersion hardening, grain-boundary strengthening, and so forth) when the interaction of single dislocations, averaged out by the continuum method, becomes important. None the less, one would hope that an integrated treatment would include the powerful formalism of the continuum approach.

G. Ellison (*Department of Mechanical Engineering, University of Bristol, U.K.*). In many components operating at high temperatures in modern power plant there are considerable difficulties in predicting material behaviour and life. This situation arises because the deformation and fracture mechanisms are somewhat complex, often involving simultaneous creep, fatigue and environmental mechanisms. Current design codes (eg. ASME III and VIII) do not take account of the actual mechanisms and in my view can lead to large errors of prediction. For example, codes effectively imply that you can simply add a transgranular fatigue and intergranular creep damage; I find this difficult to accept.

Hence I fully support what Professor Ashby calls the atomistic approach. Being an engineer I wish to predict a result, say life or stress response, numerically. To do this it must be a self-evident truth that the mechanisms régime in which we are operating must be known. I find the strength of Professor Ashby's approach is that it gives me a global view of a complex situation and in effect helps me 'select the correct' equations for use. In particular at Bristol we have attempted to use this approach to predict creep and fatigue interaction behaviour. Professor Ashby in his talk did not discuss this type of situation when combinations of behaviour can occur. I would be interested to hear his views.

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M. F. Ashby. Professor Ellison's question goes one stage beyond the problem I have addressed. The individual classes of behaviour he mentions (creep, fatigue, environmental interaction) each involve a number of mechanisms, and this complexity has hindered the development of a good engineering approach to each one. Professor Ellison asks how their interaction can be modelled. I would hope that an extension of the general approach that I have described might be capable of doing this. It is a very challenging problem.

Y. Lindblom (*FFV Materials Technology, Linköping, Sweden*). In an inspiring paper, Professor Ashby has made the first systematic effort I have known, to knit together the continuum approach of mechanical-properties description with the atomistic approach of materials-structure description. This has been a dream for the material scientists for a long time. Commercial and political decision makers demand higher reliability in complicated constructions and have a tendency to blame technology instead of insufficient economical support of reliability efforts, the result being that new materials and technology become suspect and increasingly difficult to introduce on the market.

If not complementary to the unification of the continuum and atomistic approaches, much more work also must go into further development of the probalistic approach. Not much has been done in this direction since Waloddi Weibull presented his work nearly 50 years ago.

M. F. Ashby. I agree with Professor Lindblom that the probabilistic approach in engineering design is one with great potential. As materials are pushed towards their limit, the statistical variation in their properties becomes more apparent. Always, one is working on the tail of the distribution, where the probability of failure is very small. There is urgent need for research on predicting the failure probabilities under these extreme conditions.

R. W. Cahn (*Department of Metallurgy, University of Cambridge, U.K.*). There is an invisible college of continuum plasticity experts, scattered in universities around the world, who have for decades studied the plastic behaviour of materials, metals especially, without any reference to their microstructure, not even the grain structure of polycrystals. They neither know nor care about deformation maps or structurally based constitutive equations. Sir Geoffrey Taylor, 50 years ago, first tried to relate the continuum approach to plasticity to microstructure, in his famous attempt to estimate how many slip systems were needed for any grain in a polycrystal to follow the strain externally imposed on that polycrystal. That attempt has had very few successors in the 50 years up to now; Professor Ashby is the shining exception! Does he have an explanation for this persistent standoff between the continuum people and those who pursue atomistic mechanisms?

M. F. Ashby. I think the barrier that Professor Cahn identifies arises from the complexity of real materials. Continuum mechanics is based on idealizations of elastic, plastic and creep behaviour, which in realilty are seldom realized. I think, however, that the gap between the continuum mechanicians and the materials scientists is narrowing rapidly, and is bridged at a number of points. Considerable credit for this must go to the American funding agencies that have, for some years now, insisted on an interdisciplinary approach to materials problems. The ARPA Laboratories, succeeded by the MRLs, and new URIs all have, as a guiding principle, the cooperative efforts of materials scientists, continuum mechanicians, and solid-state

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physicists. In Europe, we have been less conscious of the gains to be made from such collaborations, and are perhaps behind the U.S.A. in achieving them.

J. F. Barnes (*Ministry of Defence, London, U.K.*). If it does prove possible to develop methods, as Professor Ashby has suggested, which allow us to predict the behaviour of engineering materials in a more fundamental fashion, is it likely that we will be able to specify the composition of the material to be used in a more informed fashion? Creep, for example, is sensitive to changes in composition. In designing a component for a certain life in service, does he believe that we will be able to deduce and hence specify the permissible limits within which composition may be allowed to vary? I ask this because unnecessarily tight control of composition usually must lead to excessive cost of manufacture.

M. F. Ashby. I think it may, by using the methods I have described, be possible to identify permissible limits on the compostion of alloys, as Mr Barnes suggests. There is more scope for optimization when material properties vary continuously with some internal parameter. Composites are the obvious example. Here, the modulus, the strength and the toughness vary in a systematic way with the volume fraction and lay-up of the fibres. Then, when a set of properties is specified, it should be possible to specify a range of volume fraction of fibres, and lay-ups that would meet the specification. It is rather more difficult to do with metallic alloys, which (because of the limitations imposed by the phased diagram, and by the chemical and physical effects of the alloying element) tend to have discrete compositions, and discrete, associated properties that cannot be varied in a continuous manner.

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