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Review: The Theoretical Strength of Solids

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In principle, there is an upper limit to the mechanical strength of any material under given test conditions. This limit is called the ideal strength. This paper attempts to define the ideal strength so far as is presently possible. Firstly, a brief summary is given of the highest strengths obtained experimentally. Next follows a detailed account of the attempts to calculate the ideal strength from theoretical considerations. Finally, the experimental and calculated results are compared, and it is concluded that in one or two instances the ideal strength has probably been realised experimentally.

1. Introduction

As greater and greater mechanical strengths are obtained from engineering materials it is only logical to ask what is the upper limit to the strength of a solid. This review is concerned with the extent to which that question can be answered today.

The maximum strength of a solid has come to be referred to as the theoretical strength, and this convention has been continued in the title of this review in order to avoid confusion. However, because this strength has probably been realised experimentally, it is suggested that the term ideal strength is more suitable, and this latter term is used in the text below.

A knowledge of the ideal strength is important to our understanding of many problems in the solid state. Thus, the ideal strength plays an important role in determining the stress distribution (and other properties) in the region at the tip of a crack. It is, therefore, one of the major factors in determining cleavage behaviour, and in determining whether a material will behave in a brittle or ductile manner [1-3]. Likewise, the ideal strength plays a role in defining dislocation core radii [4, 5] and in defining the point at which coherency breakdown occurs at a particle-matrix interface [6-8]. Knowledge of the temperature variation of the ideal shear strength, for temperatures close to the melting-point, might also provide some insight into the phenomenon of melting [9].

We should note, however, that the calculations of ideal strengths reviewed here were all made on an assumption of homogeneous deformation. Consequently, the results should strictly only be applied to problems of inhomogeneous deformation in which stress and strain vary but little over distances comparable with the range of the interatomic forces. This is not the case in the immediate region of the tip of a crack, of the core of a dislocation, or of a particle-matrix interface, for example, so that due caution must be exercised in applying the results of these calculations to such problems.

The material reviewed in this paper has been divided into three sections. Section 2 discusses the high strength data obtained experimentally. Section 3 takes up the question of the calculation of the ideal strength from theoretical considerations, and reviews the results of the published work in that area. Finally, section 4 compares the experimental and calculated results as far as is possible, and considers the question of whether the ideal strength of a solid is ever observed experimentally.

2. Experimental Measurements of Very High Strengths

2.1. Summary of Results

It has been found experimentally that the very highest strengths are mostly obtained from specimens falling into one of three loosely defined categories: (i) very small whisker single crystals; (ii) larger single crystals of materials such as silicon, germanium and alumina; (iii) silica glass rods and fibres. In each category most of the high strengths have been obtained in the same way, i.e. by the low temperature bend or tensile testing of rods or bars having highly perfect surfaces (mostly prepared by flame or chemical polishing). Such surfaces are at least optically perfect. Kelly [3] and the present author [10] have summarised much of this experimental work. Subsequently, further data have been published [11-16]. Table I lists some results.

The whisker crystals (i) are probably the most nearly perfect specimens presently available. In some cases they contain no observable defects at all; in other cases just a single, axial, screw dislocation. Their strength appears to be influenced primarily by their surface condition. A wide range of materials have been prepared as whiskers, by a variety of techniques [17], so that high strengths have been obtained from many solids in this form.

Very high strengths have only been obtained from larger crystalline specimens (ii) of silicon, germanium and alumina at low temperatures. In such materials the Peierls stress is so high as to effectively immobilise any dislocations present, and both perfect [18, 19] and imperfect (see table I) crystals can show high strength. In both cases the strength is again found to be controlled primarily by surface condition.

Specimens of silica (and other) glass rods and fibres (iii) of a wide range of sizes have also been found to be very strong. As in both previous cases the strength is found to be controlled mainly by the surface condition. Structural studies [20, 21] have shown that these materials have considerable short range order, and contain a continuous network of nearest neighbour bonds of similar geometry and comparable strength to the nearest neighbour bonds of the corresponding crystalline material. By virtue of their lack of long-range order, however, glassy materials do not contain glissile dislocations.

Most of the results quoted in table I represent an isolated highest strength value recorded in a series of experiments. In a few instances, however, consistent high strengths have been recorded, comparable with these isolated values. These data are discussed below in a little more detail.

In the first such instance Crump and Mitchell [11, 16] made a series of accurate tensile measurements on cadmium whiskers. They reported that no defects of any kind were visible

TABLE I Some experimental measurements of very high strengths

Material	Maximum tensile stress σ_{max}		Reference	Remarks
	$\times 10^{-10}$ dynes/cm^2	$\frac{\sigma_{max}}{E} \approx$ strain		
(i) Whiskers				
NaCl	1.08	0.026	Gyulai [57]	$\langle 100\rangle$ tension. $\tau\{110\}\langle 1\bar{1}0\rangle = 0.54 = 0.030\,G$
Ag	1.73	0.040	Brenner [59]	,, $\tau\{111\}\langle 1\bar{1}0\rangle = 0.71 = 0.031\,G$
Cu	2.94	0.028	,,	$\langle 111\rangle$ tension. ,, $= 0.80 = 0.022\,G$
Fe	13.10	0.049	,,	,, $\tau\{110\}\langle 1\bar{1}1\rangle = 3.58 = 0.060\,G$
Cd	2.80	0.04	Crump and Mitchell [11]	$\langle 11\bar{2}0\rangle$ tension. $\tau = 0.033\text{-}0.069\,G$ for different glide systems. $\langle 10\bar{1}0\rangle$ tensile stress $= 0.026\,E$
(ii) Larger single crystals				
Ge	3.82	≈ 0.02	Johnson and Gibbs [60]	Bending, 78°K, 0.7 × 1.5 mm bar
Si	4.14	—	Gilman [61]	3.8 cm diameter ring pulled in tension
Al_2O_3	6.85	≈ 0.02	Proctor *et al* [62-64]	Bending of 1 mm diameter rods, unknown orientation
(iii) Glass rods and fibres				
SiO_2	13.1	≈ 0.18	Hillig [65]	Bend tests, 78°K, 0.5-3 mm diameter rods
SiO_2	13.8	≈ 0.19	Morley *et al* [66]	Tensile test, 77°K
(iv) Other data				
Au, Al, Cu	—	—	Gane *et al* [22-25]	Maximum shear stress $\approx 0.05\,G$
Ge	7-12	0.05-0.08	,,	Maximum shear stress $\approx$ 10-15 $\approx$ 0.2-0.3 G
MgO	5-9	0.02-0.035	,,	Maximum shear stress $\approx$ 9-15 $\approx$ 0.09-0.15 G
Cu	—	—	Brown *et al* [7-8]	Maximum shear stress at 873°K $\approx 0.039\,G$

E, G are the appropriate Young's and shear moduli. $\tau\{hkl\}\langle UVW\rangle$ is the largest component of σ_{max} on any plane of the type $\{hkl\}$ in any direction of the type $\langle UVW\rangle$.

either in the interior or on the surface of their whiskers, by means of either optical or electron microscopy. An interesting feature of their work was that, at fracture, their crystals did not shatter into many fragments as is usual at very high strengths, but only into two halves [16]. Thus, it could be determined that half their crystals failed by cleavage across a $\{10\bar{1}0\}$ plane, yielding apparently atomically smooth fracture surfaces, and leaving no traces of any dislocations in the broken parts. The remaining crystals failed by shear on various glide systems, yielding slightly ragged fracture surfaces, and leaving a few dislocations in the fracture zone. The strength values quoted in table I were calculated from Crump and Mitchell's data by the present author.

Two other such instances do not fall into any of the three categories outlined above. In one case Gane and various co-workers [22-25] used a very small scale indentation technique to study the strength of specimens of gold, copper, aluminium, germanium and magnesium oxide. However, due to the possible inaccuracies in calculating the stresses under the indenter, no great significance should be attached to the values quoted in table I. Also, since the stress distribution under the indenter is both complicated and markedly inhomogeneous, these results are not directly comparable with the calculated results reported in section 3.

In the other case Ashby *et al* [6] and Brown *et al* [7, 8] attempted to obtain an estimate of the ideal shear strength of copper, by measuring the stress at which interface dislocations were nucleated in a perfect region of a copper matrix immediately adjacent to a second phase particle. The former authors [6] studied the effect of hydrostatic pressure on the systems copper-silica and copper-alumina, in which the interface is incoherent. They found that dislocations were nucleated even at low applied pressures (corresponding to stresses in the matrix far less than the ideal strength) provided that the energy of the system was thereby reduced. These experiments, therefore, do not measure the ideal strength. Brown *et al* [7, 8] studied the system copper-cobalt, and found that large coherent precipitates could be obtained by ageing the quenched alloy at 873° K. This result suggests that the ideal shear strength of copper at 873° K is greater than the maximum shear stress generated at the particle-matrix interface (estimated to be $0.039G$ where G is the appropriate shear modulus). As in the case of the indentation experiments, however, the calculated stress is of uncertain accuracy, and the stress distribution is markedly inhomogeneous. These data, therefore, are also not directly comparable with the calculated results reported in section 3.

2.2. Interpretation of Results

In the case of both crystalline and glassy solids it is accepted that the interatomic cohesive forces are exceedingly strong, and that the presence of glissile dislocations and/or tiny cracks (most frequently initiated at surface heterogeneities) is the main cause of the relative weakness of most specimens.

Since even a single such defect can drastically reduce the strength of a specimen, and since such defects occur on a more or less statistical basis, it is also explained why very high strength, in all materials, is normally such a structure-sensitive and non-reproducible property, and why it is most frequently observed in very small specimens.

Such an understanding of mechanical properties suggests that, for any material, the strength increases with increasing structural perfection and, consequently, that the ideal strength will only be realised when the greatest possible perfection is attained. There are, however, certain limits to the degree of structural perfection attainable in a given specimen.

For crystalline specimens a limit is imposed firstly by thermodynamic considerations. An unstressed crystalline solid at thermodynamic equilibrium contains certain defects, e.g. lattice vibrations, a certain concentration of vacancies, etc. Such defects are necessarily present in any specimen. In contrast, under the same conditions, other sorts of defects, e.g. dislocations, would not be expected to occur. However, when the solid is deformed its thermodynamic potential is changed, as are the energies of formation of each kind of defect. At strains corresponding to the highest strengths these changes could conceivably be quite large. Under such conditions, therefore, the equilibrium concentrations of the different kinds of defects already present must change, and it is also conceivable that the presence of additional different kinds of defects in the solid could become thermodynamically favourable. The extent to which such changes would actually occur, in a given test, would depend on such test conditions as temperature and strain rate, which thus impose a second limit on the degree of perfection that may be obtained.

It is thus apparent that the ideal strength, like the strength measured in any experiment, is a function not only of the particular material under test, but also of the testing procedure. Thus, this strength is a function of specimen geometry, mode of deformation, temperature, strain rate, type of loading (e.g. dead loading, pressure loading etc.) imposed by the loading device, and so on.

In so far as it represents a region where the regular atomic array is disrupted, the surface of a solid may also be regarded as a defect. (This raises the question of whether the surface of a solid is inherently weaker than the interior.) In a real test the demands of specimen geometry define a certain surface orientation and a certain surface to volume ratio. The requirements of thermodynamic equilibrium, however, will generally require different values of these parameters and, moreover, values that change as the specimen is deformed. Thus, again the requirements of a practical test are incompatible with those of thermodynamic equilibrium, and hence influence both the attainable degree of crystal perfection and the ideal strength.

For amorphous specimens, which by their very nature are never in thermodynamic equilibrium anyway, the details of the preceding arguments must differ, but the same general conclusion can be drawn – namely that the requirements of a practical test procedure are likely to influence the attainable degree of specimen perfection, and hence the ideal strength.

The question now arises of whether, in any of the series of high strength measurements made under constant test conditions, the highest strength value measured was actually the ideal strength for those conditions. An attempt is made to answer this question in section 4, by comparing the experimental data discussed in this section with the results of the calculations presented in the next section.

3. Calculations of the Ideal Strength

3.1. General Considerations

In principle the methods of quantum mechanics and quantum statistical mechanics enable the ideal strength of a material to be calculated for given test conditions.

A material specimen under test consists of a finite three-dimensional array of mutually interacting atoms, that are acted on by some distribution of surface forces, and make small oscillatory motions about their equilibrium positions. A complete description of this dynamic atomic system contains all the information necessary to calculate the macroscopic properties (thermodynamic observables). In principle such a calculation proceeds from the definition of a system Hamiltonian and solution of the corresponding Schrödinger equation, to calculation of a partition function and the conventional thermodynamic potentials. Finally, the macroscopic physical properties are obtained from these potentials. Thus, for example, the state of stress in the body can be obtained as the appropriate derivative, with respect to strain, of either the internal energy or the Helmholtz free energy. The equilibrium and stability of the system require that there be no net force on each atom, and that the total system potential energy be a minimum; or equivalently, that the appropriate thermodynamic potential be a minimum. Note that these are requirements on the total system potential, which includes a contribution from the work done, in any virtual displacement, by the applied surface forces. Thus, such an analysis reflects the dependence of the strength properties of the material on the test conditions.

In practice there are two major difficulties in the scheme of calculation outlined above. The first is the lack of a sufficiently detailed knowledge of the interatomic forces to enable the correct Hamiltonian to be employed, and the second is the complexity of the calculations involved. In recent years the advent of high-speed digital computers has gone some way towards removing the latter difficulty. Due to these difficulties, however, none of the calculations of ideal strengths made to date, and reviewed in the following pages, is in any way rigorous. Thus, for example, in no case is the dynamic nature of the atomic system taken into account, but rather the static lattice potential energy (the largest contribution) is tacitly assumed equal to some thermodynamic potential – which one it is often not clear, as the test conditions are rarely precisely specified. Likewise, where lattice sums have been performed, they have invariably been performed only over atoms situated at their equilibrium positions in the interior of the solid. Thus, surface effects, thermal displacements, lattice vacancies etc have not been taken into account. Consequently, the theoretical calculations represent a best approximation at 0° K, when zero point motion is the only internal defect neglected. Also, the calculations can throw no light on the question of whether the surface of a solid is inherently weaker than the interior. Only in a few cases [10, 26, 27] has any attempt even been made to study the stability of the deformed solid. Other authors tacitly assume stability throughout the range of deformation under consideration.

3.2. Calculations Relating the Ideal Strength to Other Physical Properties

One way to circumvent the lack of knowledge about the cohesive forces, and other difficulties, is to attempt to relate the ideal strength of a solid directly to other macroscopic physical properties. Thus, Polanyi [28] and Orowan [29-31], and subsequently other authors, obtained a rough estimate of the ideal uniaxial tensile strength $\sigma_{\max}$ in terms of the equilibrium surface energy γ and interplanar spacing a_0 of the planes perpendicular to the tensile axis, and the appropriate Young's modulus E. Such an approach is equally applicable to any solid. Details of the analyses vary, but the essential assumptions are: (i) that when a tensile specimen is extended uniaxially the resulting stress-displacement curve has a simple analytical form (e.g. Johnston [32] and Kelly [3] assumed a sine curve, chosen to give the correct modulus at zero strain); (ii) that $\sigma_{\max}$ is represented by the maximum value of this curve; (iii) that the work done on the body (i.e. the change in system potential, or the stored elastic strain energy) in raising the stress to the maximum level is 2γ per unit area of atomic plane normal to the tensile axis. This latter assumption has been discussed in detail elsewhere [10]. Kelly's analysis [3] gives

$$\sigma_{\max} = \left(\frac{E\gamma}{a_0}\right)^{1/2}. \qquad (1)$$

From this equation Kelly obtained the values given in table II. The data used are appropriate to 293°K, except for those in brackets which refer to 0°K [1, 2].

In a report by the US National Academy of Sciences [33] the same calculation was used to estimate $\sigma_{\max}$ for silica glass as 2.8×10^{11} dynes/cm^2, or $\sim 0.4\,E$.

The same authors [33] have repeated the Orowan-Polanyi calculation, using a more general stress-displacement function containing three adjustable parameters. The three parameters were calculated from appropriate surface energy, thermal expansion and elastic constant values. $\sigma_{\max}$ was taken to be the maximum value of the particular stress-displacement function defined by these values. As before, the analysis can be applied equally well to any material. Different reasonable functions were found to give a spread of about 2× in the values of $\sigma_{\max}$, which is perhaps some guide to the sort of accuracy to be expected from this approach.

By means of a somewhat similar approach McClintock and O'Day [34] estimated the ideal tensile strength for triaxial tension (i.e. volume expansion) as a fraction of the bulk modulus. These authors assumed a stored elastic strain energy U that was a function only of some characteristic radial length r, so that

$$U = A\left[(r_0/r)^m - \frac{m}{n}(r_0/r)^n\right] \qquad (2)$$

where A and r_0 are constants. The ideal strength was taken to be the maximum value of $\partial U/\partial r$. For the case $n = 1$ they showed that, as m changed from 3 to 13, so the ratio of the ideal strength to the bulk modulus fell from 0.074 to 0.039.

As in the preceding cases this last treatment is

TABLE II Simple calculations of the ideal tensile strength $\sigma_{\max}$

Material	Tensile direction	$E \times 10^{-11}$ dynes/cm^2	γ ergs/cm^2	$\sigma_{\max} \times 10^{-11}$ dynes/cm^2	$\frac{\sigma_{\max}}{E}$
Ag	⟨111⟩	12.1	1130	2.4	0.20
Au	⟨111⟩	11.0	1350	2.7	0.25
Cu	⟨111⟩	19.2	1650	3.9	0.20
Cu	⟨100⟩	6.7 (7.5)	1650 (3630)	2.5 (3.87)	0.37 (0.51)
W	⟨100⟩	39 (40.5)	3000 (6415)	6.1 (9.08)	0.16 (0.22)
α-Fe	⟨100⟩	13.2 (14.3)	2000 (4520)	3.0 (4.79)	0.23 (0.34)
α-Fe	⟨111⟩	26.0	2000	4.6	0.18
Si	⟨111⟩	18.8	1200	3.2	0.17
C (diamond)	⟨111⟩	121	5400	20.5	0.17
SiO_2 (glass)	—	7.3	560	1.6	0.22
NaCl	⟨100⟩	4.4	115	0.43	0.10
MgO	⟨100⟩	24.5	1200	3.7	0.15
Al_2O_3	⟨0001⟩	46.0	1000	4.6	0.10

not particular to any one material, and in fact has been employed by Demishev and Bartenev [35, 36] to obtain an estimate of 7.83×10^{11} dynes/cm^2 for the ideal strength of silica glass in triaxial tension.

Frenkel [37] also used a similar method to estimate the ideal shear strength $\tau_{\max}$ of a solid subjected to a simple shear mode of deformation. He assumed that, for any solid, the shear stress τ to shear any plane a distance x over its neighbour was given by

$$\tau = K \sin \frac{2\pi x}{b} \tag{3}$$

where b is the appropriate repeat distance in the direction of shear. The planes are assumed to be undistorted by the shear. K is chosen to give the correct shear modulus G. It is then easily shown that

$$\tau_{\max} = \frac{Gb}{2\pi d} \tag{4}$$

where d is the interplanar spacing of the shearing planes. Hence, for an fcc metal in $\{111\}\ \langle 11\bar{2}\rangle$ shear, $\tau_{\max} = G/2\pi\sqrt{2}$.

Equation 3 may also be written as

$$\tau = \frac{\partial U(x)}{\partial x} \tag{5}$$

where $\tau_{\max}$ is the maximum value of τ and

$$U(x) = \frac{Gb^2}{4\pi^2 d}\left(1 - \cos \frac{2\pi x}{b}\right) \tag{6}$$

and represents the stored elastic strain energy of the bulk crystal per unit area of shear plane. Mackenzie [38] recognised that equation 6 represented the first two terms of a Fourier series, and suggested that incorporation of higher order terms in the series would give a better approximation to the stored elastic strain energy. He showed how to deduce the coefficients of the next two terms for the particular cases of an fcc crystal deformed homogeneously in $\{111\}$ $\langle 11\bar{2}\rangle$ shear and $\{111\}$ $\langle 1\bar{1}0\rangle$ shear. If it is assumed that $U(x)$ refers not to a bulk crystal, but to a crystal consisting of just two close packed atomic planes, then Mackenzie's arguments become applicable also to cph crystals of ideal axial ratio $\sqrt{(8/3)}$. Kelly [3] has further extended Mackenzie's ideas to bcc metals (for $\{110\}$ $\langle 1\bar{1}0\rangle$ shear), to cph metals with non-ideal axial ratios, to graphite, and to alumina. In all cases the estimate of $\tau_{\max}$ so obtained is very sensitive to the coefficients of the additional higher order terms. Table III lists some results obtained by Kelly [3]. Except in the one designated instance these results are computed from room temperature data. In each case G is taken to be $1/s'_{44}$ (in the notation of Nye [39]), thus allowing for the relaxation and distortion that would tend to occur during the shear process. Note that this is inconsistent with the strict geometric arguments used to obtain the coefficients of the extra terms of $U(x)$ in the first place. This analysis gives good agreement with the maximum shear strain observed in experiments with the Bragg bubble raft model of a crystal [40, 41]. The oft-quoted result that $\tau_{\max} \simeq G/30$ for an fcc metal originates from this analysis by Mackenzie.

These simple calculations can be criticised on a variety of grounds, in addition to those already mentioned. Their starting point is an empirical description of a bulk property rather than the description of the atomic system. In no case is any model of the interatomic forces taken into account explicitly and, with the exception of the work of Mackenzie and its development by

TABLE III Simple calculations of the ideal shear strength $\tau_{\max}$

Material	Shear plane and direction	$G \times 10^{-11}$ dynes/cm^2	$\tau_{\max}/G$	$\tau_{\max} \times 10^{-10}$ dynes/cm^2
Cu (10° K)	$\{111\}\ \langle 11\bar{2}\rangle$	3.32	0.028-0.039	0.93-1.29
Cu	$\{111\}\ \langle 11\bar{2}\rangle$	3.08	,,	0.86-1.20
Au	$\{111\}\ \langle 11\bar{2}\rangle$	1.90	,,	0.53-0.74
Ag	$\{111\}\ \langle 11\bar{2}\rangle$	1.97	,,	0.55-0.77
Al	$\{111\}\ \langle 11\bar{2}\rangle$	2.30	,,	0.65-0.90
Al	$\{111\}\ \langle 1\bar{1}0\rangle$	2.30	0.114	2.62
Fe	$\{1\bar{1}0\}\ \langle 111\rangle$	6.0	0.11-0.13	6.6-7.8
W	$\{1\bar{1}0\}\ \langle 111\rangle$	15.0	0.11-0.13	16.5-19.5
Al_2O_3	$\{0001\}\langle 11\bar{2}0\rangle$	14.7	0.115	16.9
Zn	$\{0001\}\langle 10\bar{1}0\rangle$	3.8	0.034*	1.3
C (graphite)	$\{0001\}\langle 10\bar{1}0\rangle$	0.23	0.05*	0.0115

*These values of $\tau_{\max}/G$ differ from 0.028-0.039 due to non-ideal axial ratios.

Kelly, neither is crystal structure an explicit factor in the calculations. Nevertheless, despite the fact that the results of these calculations can only be regarded as order of magnitude estimates, they are widely quoted. Also, the early work of Polanyi and Frenkel was historically important in emphasising the difference between the actual and the ideal strengths of solids. The need to reconcile this disparity lead in turn to the appreciation of the role of defects in determining mechanical behaviour.

3.3. Calculations of the Ideal Strength using the Morse Potential

A different but still very simple approach to calculating the ideal strength of a solid is that adopted first by de Boer [42]. This treatment attempts to remove one criticism of the work already mentioned in that it makes use of an explicit, albeit crude, model of the interatomic forces in a given material. As before, the results should only be regarded as order of magnitude estimates.

De Boer assumed that the energy of an aliphatic carbon-carbon bond, as a function of the interatomic separation, could be represented by a Morse function. The three adjustable parameters of this function were deduced from the equilibrium carbon-carbon distance, the binding energy, and a characteristic adsorption frequency, determined spectroscopically. The force required to break one such bond is just the maximum slope of the resultant Morse function. De Boer calculated this force as 5.64×10^{-4} dynes and, knowing the number of bonds per unit area (from crystallographic data), he estimated $\sigma_{\max}$, the ideal uniaxial tensile strength, of phenol formaldehyde and m-cresol formaldehyde as 4.3×10^{11} and 3.8×10^{11} dynes/cm^{2}respectively. The calculations assumed also that the straight carbon-carbon chains of these structures were continuous throughout, and aligned parallel to the tensile axis.

Tyson [43] calculated $\sigma_{\max}$ for the $\langle 111 \rangle$ direction in diamond in essentially the same way, obtaining $\sigma_{\max} = 10.6 \times 10^{11}$ dynes/cm^2.

Likewise, by applying the same analysis to the pseudo-diatomic molecule SiO_3-O, Ladik and Naray-Szabo [44] estimated $\sigma_{\max}$ for silica glass as 2.42×10^{11} dynes/cm^2.

The same approach has been extended to zigzag carbon-carbon chains (e.g. polymethylene), where simultaneous bending and stretching of the bonds occurs [33]. In this work a Morse function model of the stretching of the bonds was combined with an empirical model of the bending of the bonds to obtain a potential energy-displacement function. This function gave a smooth stress strain curve, and was consistent with the binding energy and equilibrium stereochemistry of the chain, the inversion energy, and the spectroscopically determined force constants for bending and stretching of the bonds of the chain. From this model the ideal uniaxial tensile strength $\sigma_{\max}$ parallel to the carbon-carbon chains was estimated as 3×10^{11} dynes/cm^2 (at a strain ~ 0.3).

The same authors made a few qualitative attempts to extend this argument to other carbon-carbon structures. One example of interest is graphite, where $\sigma_{\max}$ in any direction in the basal plane was estimated to be $\sim 17 \times 10^{11}$ dynes/cm^2. Due to its layer structure graphite may also be expected to show high strength in biaxial loading, in contrast to the chain structures.

Tyson [43] employed a similar potential model to calculate $\tau_{\max}$ for diamond in $\{111\}$ $\langle 1\bar{1}0 \rangle$ simple shear. He considered the change in energy of a carbon atom during shear due both to the bending and the stretching of the bonds with its nearest seven neighbours. He also assumed the stretching to be described by a Morse function. The bending he described by an empirical function that took into account the fact that the resistance to bending decreased with increasing bond length. He then calculated $\tau_{\max}$ from the product of the derivative of the energy per atom with respect to the shear strain and the number of carbon atoms per unit area, obtaining 9.16×10^{11} dynes/cm^2 at a shear strain of 0.29.

Recently Milstein [27] has used a Morse potential function to calculate the ideal $\langle 100 \rangle$ unconstrained uniaxial tensile and compressive strengths of bcc α-iron. For the adjustable parameters in the model Milstein used values determined originally by Girifalco and Weizer [45] from the bulk compressibility, the binding energy, and the equilibrium lattice parameter. Milstein employed computational methods very similar to those used by the present author [10], by Born and Fürth [26], and by Tyson [43] in their calculations with the Lennard-Jones and Born-Mayer potentials (see sub-sections 3.4.2 and 3.4.3). Like the present author [10] and Born and Fürth [26], Milstein also investigated the stability of the deformed crystal, assuming dead loading conditions. In discussing Milstein's results here the same notation as is to be used in sub-sections 3.4.2 and 3.4.3 is employed, for the sake of consistency, even though this has not yet been defined.

Thus, for bcc α-iron Milstein found that in tension the deformation remained stable almost up to the maximum value of σ_{33} of 1.7×10^9 dynes/cm^2 at a strain $c_{33} = 0.017$. Hence, very little error would arise in this case from assuming the deformation to be stable up to the maximum value of σ_{33}, and equating the ideal strength to this value. In compression the first instability occurred at $\sigma_{33} = -5.05 \times 10^9$ dynes/cm^2, $c_{33} = -0.016$.

The present author [10] also investigated this same potential model, and found that it predicted the stable form of iron to be an fcc structure having a nearest neighbour distance ~3% larger than that in the equilibrium bcc form. A postulated cph polymorph, with the same larger nearest neighbour distance and ideal axial ratio, had a binding energy only fractionally higher than the fcc form. Milstein, however, found that the model predicted that a body-centred tetragonal (bct) form, having c and a lattice parameters of 1.26 and 0.89 times the bcc lattice parameter respectively, would have a binding energy ~0.02% lower than the fcc form. For this postulated structure he found that, in ⟨001⟩ tension, the first instability occurred at $\sigma_{33} = 8.90 \times 10^{10}$ dynes/cm^2 at a strain $c_{33} = 0.071$. In this case the ideal strength is far less than the maximum value of σ_{33} which he calculated as 4.44×10^{11} dynes/cm^2. In compression Milstein found the first instability at $\sigma_{33} = -3.22 \times 10^{10}$ dynes/cm^2, $c_{33} = -0.074$.

3.4. Calculations of the Ideal Strength of Van der Waals and Ionic Solids

3.4.1. Introduction

Calculations of the ideal strength from more realistic models of the interatomic forces have only been made for van der Waals and ionic solids, in which these forces are best understood. Even in these cases, however, the available models of the interatomic forces are only approximate.

It is not intended to give here a review of interatomic potential models. Rather, the interested reader is referred in the first instance to reviews of van der Waals bonding by Pollack [46] and Winterton [47], and of ionic bonding by Tosi [48].

For present purposes it is sufficient to note that the procedure adopted in all of the work discussed here has been to obtain a reasonable approximation to the analytical form of the major contributions to the interatomic potential, and then to introduce (say) n adjustable parameters into this approximate function. The values of these n parameters are then computed from the experimentally measured values of n physical properties, and the resulting model used to calculate the required $(n + 1)^{\text{th}}$ property (i.e. the ideal strength). In this way it is hoped that the various errors in the potential model will tend to cancel each other out. Clearly, if the $(n + 1)^{\text{th}}$ property is closely related to the other n the calculation is more likely to yield a reliable result. However, easily measurable structure insensitive physical properties tend to depend on the shape of the bottom of the potential energy well that each atom occupies in the lattice, while the ideal strength tends to depend on the maximum slope of the side of this potential well. Thus, ideal strengths are not closely related to other easily measured properties, and the calculated values of these strengths are of uncertain accuracy.

The potentials that enter into the present discussion – i.e. the Lennard-Jones model of van der Waals solids, and the Born and Born-Mayer models of ionic solids – are both spherically symmetric, two-body, central force potentials. As such they are most reliably applied to structures of high symmetry, and tend to become increasingly unreliable as the strain increases, symmetry decreases, and the constituent atoms become polarised. Due to the relatively much weaker nature of the interatomic forces in a van der Waals solid as compared to an ionic solid, it is likely that polarisation is rather more serious in the latter case, and the calculated ideal strengths accordingly less reliable.

3.4.2. Van der Waals Solids

The first estimates of the strength of van der Waals forces were made by de Boer [42] in the course of his studies, described above, of m-cresol and phenol formaldehyde polymers. The major contribution to van der Waals binding is due to dipole-dipole interactions, which give rise to an interaction energy depending on the inverse sixth power, and a force of attraction depending on the inverse seventh power, of the distance between the atoms. Using this model of the attractive forces, and assuming that the repulsive forces per unit area between two planes were proportional to the inverse tenth power of the interplanar distance, de Boer made two different estimates of a lower limit to the ideal tensile strength of the van der Waals forces between the carbon-carbon chains of m-cresol formaldehyde and phenol formaldehyde polymers. The first estimate gave values of 6.4 and 8×10^8 dynes/cm^2 respectively, and the second, which de Boer considered a better estimate, gave values of 3.2 and 3.9×10^9 dynes/cm^2 respectively. De Boer also made a calculation of the contribution of van der Waals forces to the ideal tensile strength of sodium chloride (see subsection 3.4.3 below).

Subsequently, Mackenzie [38], Tyson [43], Born and Fürth [26], and the present author [10] have all made estimates of the ideal strength for various modes of homogeneous deformation of a monatomic fcc van der Waals solid, using the Lennard-Jones 6-12 potential model. The discussion of this work given here is taken from [10], and is essentially a more formal and general statement of the method used by Tyson [43]. Both authors used a computer to perform all lattice summations, and the minor discrepancies between their results are due only to differences in computational procedures.

In the Lennard-Jones potential model the energy of interaction $u(R)$ of some arbitrary origin atom in the interior of the deformed crystal with some other interior atom at position X_i is given by

$$u(R) = A\left[\frac{B}{R^{12}} - \frac{1}{R^6}\right] \qquad (7)$$

where

$$R = (X_i X_i)^{1/2}\,. \qquad (8)^*$$

The total energy of the origin atom is given by

$$U = \tfrac{1}{2}\sum_R u(R) \qquad (9)$$

where $\sum_R$ runs over all the atom positions in an (interior) region surrounding the origin atom. Since the deformation is homogeneous and surface effects are neglected, U is independent of the choice of origin atom and can be regarded as the energy of the whole crystal, expressed per atom. The present author typically included a few hundred atoms in each summation $\sum_R$, giving a convergence error in the calculated value of the ideal strength of $< 1\%$ [10]. Further details of the different summation and other computational procedures used by the several authors can be found in the original references [10, 26, 38, 43].

If the atom at X_i in the deformed crystal was at x_i in the unstrained state, so that the homogeneous deformation is described by the non-symmetric second-rank strain tensor c_{ij} defined by

$$X_i = x_i + c_{ij}x_j \qquad (10)^*$$

then it can be shown that the corresponding symmetric stress tensor σ_{ij} is given by

$$\sigma_{ij} = \frac{n}{2v}(\delta_{jk} + c_{jk})\sum_R\left[\frac{X_i x_k}{R}\frac{\partial u(R)}{\partial R}\right] \qquad (11)^*$$

where δ_{ij} is the Kronecker delta, n the number of atoms in one unit cell, and v the volume of one unit cell in the deformed crystal.

The present author [10] has calculated the ideal strength of solid argon from these equations for a wide variety of different modes of deformation, using appropriate values of A and B (equation 7) computed from the lattice parameter and binding energy at 0° K [49]. The most important results from [10] are summarised below in table IV. Also included in that table for purposes of comparison are a summary of the results of Mackenzie, Born and Fürth, and Tyson. These authors all used arbitrary units, so that only their values of geometric parameters and of the ratios σ_{max}/E or τ_{max}/G make meaningful comparisons. Consequently only this information is included in table IV. Table V lists the elastic constants of argon calculated by the present author from the same potential model, together with the experimentally determined values. The comparison of these values affords one test of the validity of the potential model.

Several comments are needed to amplify table IV. The labels (*a*)-(*j*) used below correspond to the same labels in table IV itself.

(*a*) In uniaxial tension Ox_3 is arbitrarily chosen as the tensile axis. Thus, for constrained tension all c_{ij} are zero except c_{33}, and for unconstrained tension all σ_{ij} are zero except σ_{33}.

(*b*) In each case the ideal strength is taken to be the largest value of σ_{33}–i.e. it is implied that the deformation remains stable up to this point–and the strain values quoted are those corresponding to this stress.

(*c*) This direction, between $\langle 110\rangle$ and $\langle 100\rangle$, and about 5° from the former, corresponded to the lowest value of σ_{max} for constrained uniaxial tension. $\langle 111\rangle$ gave the highest value.

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*In equations marked thus * the Einstein summation convention is implied.

TABLE IV The ideal strength of solid argon (units of 10^{10} dynes/cm^2)

Mode of Deformation	σ_{max} (*b*)	c_{33}	$c_{11} = c_{22}$	E	σ_{max}/E	Author
Uniaxial tension (*a*)						
$\langle 100\rangle$ constrained	0.320	0.23	0	3.86	0.083	Macmillan
$\langle 110\rangle$,,	0.268	0.20	0	5.24	0.051	,,
$\langle 111\rangle$,, (*c*)	0.345	0.18	0	5.70	0.061	,,
$\langle hol\rangle$,, (*c*)	0.267	0.20	0	—	—	,,
$\langle 100\rangle$ unconstrained (*d*) (*e*)	0.345	0.26	− 0.027	2.24	0.154	,,
,,	—	$\frac{(1+c_{33})}{(1+c_{11})} \approx 1.25$		—	0.16	Born and Fürth
,,	—	0.25	—	—	0.145	Tyson
$\langle 111\rangle$ unconstrained (*d*) (*e*)	0.352	0.18	− 0.006	5.20	0.068	Macmillan
,,	—	0.18	—	—	0.064	Tyson
Biaxial tension and plane strain (*f*)	0.256 (*f*)	0	0.13	—	—	Macmillan
Triaxial tension (*g*)	0.254 (*g*)	0.09	0.09	—	—	,,
	τ_{max} (*i*)	c_{31}	c_{11} (*j*)	G	τ_{max}/G	
Simple shear (*h*)						
plane direction						
$\{100\}$ $\langle 001\rangle$	0.243	0.20	0.088	—	—	Macmillan
$\{100\}$ $\langle 011\rangle$	0.196	0.16	0.055	—	—	,,
$\{110\}$ $\langle 001\rangle$	0.425	0.22	0.077	—	—	,,
$\{110\}$ $\langle 1\bar{1}0\rangle$	0.261	0.34	0.051	—	—	,,
$\{111\}$ $\langle 1\bar{1}0\rangle$	0.137	0.20	0.044	—	—	,,
$\{111\}$ $\langle \bar{1}\bar{1}2\rangle$	0.188	0.20	0.058	—	—	,,
$\{111\}$ $\langle 11\bar{2}\rangle$	− 0.077	− 0.12	0.015	1.043	0.074	,,
,,	—	− 0.13	—	—	0.062	Tyson
,,	—	− 0.13	—	—	0.062	Mackenzie

TABLE V The elastic constants of argon*

	Calculated	Experimental		
c_{11}	3.86	4.39	5.29	4.82
c_{12}	2.21†	1.83	1.35	1.28
c_{44}	2.21†	1.64	1.59	1.24
Temperature °K	0	0	4.2	0
Reference	[10]	[67]	[68]	[69]

*In the notation of Nye [39], units of 10^{10} dynes/cm^2.
†These values are required to be equal by the Cauchy relations.

(*d*) The values of c_{11} ($= c_{22}$) corresponding to $\sigma_{11} = \sigma_{22} = 0$ were found by minimising the crystal energy with respect to c_{11} for each value of c_{33}. For less symmetric orientations of Ox_3 a minimisation with respect to more than one parameter is required (see [10] for further details).

(*e*) In the unconstrained calculations Poisson's ratio was found to decrease steadily with increasing c_{33}, and even to change sign at very high stress levels. Thus, at the highest stresses, the crystal expanded rather than contracted laterally with increasing tensile strain.

(*f*) This mode of deformation is defined by $\sigma_{11} = \sigma_{22} \neq 0$, $c_{33} = 0$, where Ox_i are the cube axes. Hence $c_{11} = c_{22} \neq 0$, $\sigma_{33} \neq 0$, and all off diagonal c_{ij} and σ_{ij} are zero. The value quoted for σ_{max} is the maximum value of σ_{11} ($= \sigma_{22}$).

(*g*) This mode of deformation is defined by $\sigma_{11} = \sigma_{22} = \sigma_{33} \neq 0$. Hence $c_{11} = c_{22} = c_{33} \neq 0$, and all off diagonal c_{ij} and σ_{ij} are zero. The value quoted for σ_{max} is the maximum value of σ_{11}($= \sigma_{22} = \sigma_{33}$).

(*h*) Calculations of the ideal strength in simple shear τ_{max} are inherently more difficult, since shear in even the most symmetrical directions considerably reduces crystal symmetry [10]. Thus, several parameters are needed to fully relax the crystal. In the present calculations the convention was adopted of shearing parallel to Ox_3, on the plane perpendicular to Ox_1. Thus, a shear strain c_{31} was imposed, and the shearing planes (which were assumed to be rigid) were then allowed to relax parallel to Ox_1 – i.e. the energy of the crystal was minimised with respect to c_{11} for each value of c_{31}. This is the most important relaxation, and has the most marked effect on τ_{max}. It is important to recognise here, however, that quite large stresses remain unrelaxed, so that the values of τ_{max} quoted are probably overestimates.

(*i*) The value quoted for τ_{max} is the maximum value of σ_{31}.

(*j*) The spacing of the shearing planes was found to increase ever more rapidly with increasing c_{31} until, at the largest shear strains, the planes were moving apart normally as much as they were sliding over one another.

It is also interesting to note that σ_{max} and the corresponding value of c_{33} for constrained uniaxial tension showed comparatively little variation with orientation. Also, the differences between the σ_{max} values for constrained and unconstrained uniaxial tension in given high symmetry directions were small. It is therefore concluded that the ideal strength of argon for unconstrained uniaxial tension in any direction is also likely to show little orientation dependence. It is also seen from table IV that, in the shear calculations, the increase in interplanar spacing of the shear planes is least for $\{111\}$ $\langle 11\bar{2}\rangle$ shear. This mode corresponds to the observed slip system of the fcc structure, and gave the lowest value of τ_{max}. In separate calculations it has been shown [10] that for this shear mode: (i) at the strain corresponding to the quoted value of τ_{max} the unrelaxed stress components acting on the crystal were $\sigma_{22} = -0.053$, $\sigma_{33} = 0.070$ (in the units of table IV); (ii) over a wide range of values of σ_{11}, $\partial\tau_{max}/\partial\sigma_{11} = -0.172$.

Finally, calculations have also been made [10, 26] for the case of $\langle 100\rangle$ unconstrained uniaxial tension to test the assumption that the deformation remains stable up to the maximum value of σ_{33}. Assuming dead loading, the present author [10] concluded that the crystal will first become unstable with respect to some arbitrary virtual displacement when $\sigma_{33} = 2.9 \times 10^9$ dynes/cm^2 – i.e. the ideal strength in this mode of deformation, at least under dead loading conditions, is $\sim 15\%$ less than the maximum value of σ_{33}. The corresponding maximum strain is reduced from $c_{33} = 0.26$, $c_{11} = c_{22} = -0.027$ to $c_{33} \simeq 0.12$, $c_{11} = c_{22} = -0.024$. A similar analysis by Born and Fürth [26], in arbitrary units, predicted a similar percentage reduction in the stress values, and similar reductions in the strain values.

The present author [10] similarly examined the case of biaxial tension and plane strain, and found a reduction in the estimated ideal strength for that mode of deformation of approximately 6%, to 2.40×10^9 dynes/cm^2, and in the corresponding strain c_{11} ($= c_{22}$) from 0.13 to 0.09.

3.4.3. Ionic Solids

The ideal strength of sodium chloride has also been widely studied, using the Born and the Born-Mayer potential models. It was as long ago as 1923 that Zwicky [50] first used the former model – which may be written in the notation of the present paper as

$$u(R) = \pm \frac{e^2}{R} + \frac{A}{R^n} \qquad (12)$$

where *e* is the charge on the electron. Zwicky used a semi-analytical method to sum this energy function over all lattice sites to obtain the total energy, and to differentiate this energy to obtain the stress. He took $n = 9$ from compressibility data, and deduced *A*, which was assumed to be the same for anion-anion, anion-cation and cation-cation interactions, from the requirement that the total energy be a minimum at the observed equilibrium lattice parameter. Zwicky assumed Poisson's ratio to be constant, and the deformation to be stable up to the stress maximum – so that in effect he calculated σ_{max} as the maximum tensile stress for partly constrained $\langle 100\rangle$ uniaxial tension. He obtained $\sigma_{max} = 2 \times 10^{10}$ dynes/cm^2 at a tensile strain of 0.14 and a Poisson contraction of 0.023.

De Boer [42] repeated this calculation, without taking the Poisson contraction into account, and using a simpler, semi-analytic method of computation. He thereby estimated σ_{max} for constrained uniaxial tension as 2.83×10^{10} dynes/cm^2 at a tensile strain of 0.17. In a further version of this calculation, which incorporated a crude estimate of the van der Waals contribution to the bonding, de Boer obtained a maximum tensile stress of 2.62×10^{10} dynes/cm^2.

Tyson [43] also repeated Zwicky's Born model calculation, allowing for Poisson contraction,and performing all lattice sums accurately on a computer. He calculated σ_{max} for $\langle 100\rangle$ unconstrained tension as 2.27×10^{10} dynes/cm^2 (0.05*E*) at a tensile strain of 0.14.

More recently Bartenev and Koryak-Doronenko [51] used the same Born model to calculate the maximum tensile stress in sodium chloride deformed in $\langle 110\rangle$ and $\langle 111\rangle$ uniaxial tension. They too assumed Poisson's ratio to be constant, but to have different values in two perpendicular directions. This last assumption is in contradiction to the symmetry requirements in the case of $\langle 111\rangle$ uniaxial tension. In the $\langle 110\rangle$ case these authors obtained $\sigma_{max} = 3.86 \times 10^{10}$ dynes/cm^2 at a tensile strain of 0.185, with Poisson contractions of 0.0450 and 0.0298 parallel to $\langle 1\bar{1}0\rangle$ and $\langle 001\rangle$ respectively. For $\langle 111\rangle$ extension they obtained $\sigma_{\max} = 7.15 \times 10^{10}$ dynes/cm^2 at a tensile strain of 0.25, with Poisson contractions of 0.025 and 0.031 parallel to $\langle 1\bar{1}0\rangle$ and $\langle 11\bar{2}\rangle$ respectively. Due to the particular assumptions about Poisson's ratio, both these values of $\sigma_{\max}$ refer to partly constrained uniaxial tension.

Tyson [43] also applied the Born model to the calculation of the ideal strength of sodium chloride in simple shear. In a calculation of $\tau_{\max}$ for $\{110\}$ $\langle 1\bar{1}0\rangle$ shear, making the same assumptions about relaxation and stability as in the argon shear calculations listed in table IV and discussed earlier, Tyson obtained 2.58×10^{10} dynes/cm^2 (0.13G) at a shear strain of 0.24. By allowing suitable (uniform) distortion of the shear planes, Tyson found that this value could be reduced to 1.99×10^{10} dynes/cm^2 (0.10G) at a shear strain of 0.20.

Recently, Tyson [43], Szomor [52], Kelly, Tyson, and Cottrell [1], and the present author [10] have all used the Born-Mayer potential model to extend these calculations. In this model

$$u(R) = \pm\frac{e^2}{R} - \frac{c_{ij}}{R^6} - \frac{d_{ij}}{R^8} + bb_ib_jf_{ij}e^{-R/\rho} \qquad (13)$$

c_{ij} and d_{ij} refer respectively to the dipole-dipole and dipole-quadrupole van der Waals interactions, and each differ for anion-anion, anion-cation and cation-cation interactions. The Pauling factors f_{ij} have a similar multiplicity of values. The parameters b_i differ for anions and cations. The values of c_{ij} and d_{ij} are obtained experimentally; those of f_{ij}, b_i, b and ρ are adjustable, and are determined from the bulk compressibility, the equilibrium lattice parameter, and certain empirically observed rules about the additivity of the ionic radii in series of alkali halides. All data used by the present author were appropriate to room temperature. Further information can be found in the literature [10, 43, 48].

Szomor [52] used a computational method similar to that of Zwicky [50] to calculate the maximum tensile stress for partly constrained $\langle 100\rangle$ uniaxial tension for a range of alkali halides. He obtained a value for sodium chloride of 2.95×10^{10} dynes/cm^2.

Tyson [43], Kelly, Tyson, and Cottrell [1], and the present author [10] all used similar methods of computation that are extensions of the analysis presented in the previous sub-section 3.4.2 for argon.

It has been shown by Born and Huang [53] that, in a crystal having more than one atom per lattice point, each sub-lattice is similarly deformed if the interatomic forces are central in nature, and if each atom site is a centre of symmetry. This is the case for the sodium chloride structure, and means that no "internal strain" will occur in the unit cell of the deformed crystal. Hence the same set of strain parameters c_{ij} is sufficient to describe the deformation in this case also. Thus, to extend the previous argon calculations to the case of sodium chloride it is only necessary to generalise the summation $\sum_R$ of equations 9 and 11 to include all the different anion-anion, anion-cation and cation-cation interactions. The details are discussed fully by [10].

The maximum stress values and elastic constants obtained from these calculations are listed in tables VI and VII, which are analogues of tables IV and V respectively. In particular, the comments labelled (*a*)-(*j*) in the previous sub-section 3.4.2 are equally applicable to tables IV and VI. The following discussion, therefore, mentions explicitly only the differences in behaviour between the argon and sodium chloride cases.

In the sodium chloride case $\sigma_{\max}$ for constrained tension is a minimum parallel to $\langle 100\rangle$ and a maximum parallel to $\langle 111\rangle$. The variation in $\sigma_{\max}$ with orientation is far greater than in the argon case for both constrained and unconstrained tension. In both modes the high $\langle 111\rangle$ strength results from trying to pull apart alternate $\{222\}$ layers of anions and cations. For sodium chloride the calculation of $\sigma_{\max}$ has been carried out for $\langle 110\rangle$ unconstrained tension. This required minimising the energy of the crystal with respect to the two independent parameters c_{11} and c_{22} for each value of c_{33}.

In many modes of deformation the effect of relaxation is greater in the sodium chloride case than in the argon case (e.g. for sodium chloride in $\{110\}$ $\langle 1\bar{1}0\rangle$ shear, it has been shown [1, 10] that $\partial\tau_{\max}/\partial\sigma_{11} \simeq -0.5$). Note too that although the value of $\tau_{\max}$ for $\{110\}$ $\langle 1\bar{1}0\rangle$ shear, which corresponds to the observed glide elements in sodium chloride, is the lowest for a shear that regenerates the crystal lattice, it is not the lowest value found overall. It is not possible to judge whether the results of the fully relaxed calculations would change this situation. In one case, $\{110\}$ $\langle 001\rangle$ shear, the shearing planes get

TABLE VI The ideal strength of sodium chloride (units of 10^{11} dynes/cm^2)

Mode of deformation	$\sigma_{\max}$	c_{33}	$c_{11} = c_{22}$	E	$\sigma_{\max}/E$	Author
Uniaxial tension						
⟨100⟩ constrained	0.282	0.17	0	4.616	0.062	Macmillan
,,	0.300	—	0	4.98	0.06	Tyson
⟨110⟩ constrained	0.596	0.34	0	4.873	0.122	Macmillan
⟨111⟩ constrained	2.009	1.77	0	4.945	0.405	,,
⟨100⟩ unconstrained	0.240	0.18	− 0.031	3.682	0.065	,,
,,	0.266	0.13	—	4.08	0.067	Tyson
⟨110⟩ unconstrained	0.461	0.29	$c_{22} = -0.083$ $c_{11} = 0.005$	4.078	0.113	Macmillan
⟨111⟩ unconstrained	1.240	0.42	− 0.024	4.204	0.295	,,
Biaxial tension and plane strain	0.350	0	0.16	—	—	Macmillan
,,	0.363	0	—	6.55	0.055	Tyson
Triaxial tension	0.428	0.16	0.16	—	—	Macmillan
,,	0.434	—	—	8.04	0.054	Tyson
	$\tau_{\max}$	c_{31}	c_{11}	G	$\tau_{\max}/G$	
Simple shear						
plane direction						
{100} ⟨001⟩	0.419	0.30	0.075	—	—	Macmillan
{100} ⟨011⟩	0.353	0.30	0.056	—	—	,,
,,	0.360	0.30	—	1.64	0.217	Tyson
{110} ⟨001⟩	1.762	0.60	− 0.051	—	—	Macmillan
{110} ⟨1$\bar{1}$0⟩	0.267	0.30	0.091	1.454	0.183	,,
,,	0.284	0.27	—	1.72	0.164	Tyson
{111} ⟨1$\bar{1}$0⟩	0.320	0.44	0.109	—	—	Macmillan
{111} ⟨$\bar{1}\bar{1}$2⟩	0.229	0.28	0.054	—	—	,,
{111} ⟨11$\bar{2}$⟩	− 0.510	− 0.60	0.021	—	—	,,

TABLE VII The elastic constants of sodium chloride*

	Calculated	Experimental
c_{11}	4.616	4.87
c_{12}	1.707†	1.24
c_{44}	1.707†	1.26
Temperature °K	300	300
Reference	[10]	[70]

*In the notation of Nye [39], units of 10^{11} dynes/cm^2.
†These values are required to be equal by the Cauchy relations.

closer together initially and, although they start to separate at larger shear strains, they never regain their original spacing. This is due to the fact that initially each ion moves towards one of the opposite sign in the layer below.

The order of magnitude increase in both elastic constants and maximum stress values for sodium chloride, over the corresponding values for argon, is simply a measure of the much greater strength of the ionic bond.

The results show that for ⟨100⟩ tension there is reasonable agreement between the values obtained from the Born potential and those obtained from the Born-Mayer potential. For ⟨110⟩ and ⟨111⟩ tension the agreement between the calculations of the present author [10] (Born-Mayer potential) and those of Bartenev and Koryak-Doronenko [51] (Born potential) is less good. These discrepancies can probably be traced to the particular constraints imposed by the values of Poisson's ratio assumed by the latter authors. In the case of the shear calculations agreement between the results obtained from the two potentials is again quite good.

Using the same analysis as in the case of the argon calculations, the present author [10] has made a few investigations of the validity of the assumption that the deformation of sodium chloride remains stable up to the maximum value of the appropriate stress component. For ⟨100⟩ constrained tension it was found that the ideal strength was predicted to be 2% less than the maximum stress (with a corresponding reduction in c_{33} from 0.17 to 0.14), while for ⟨100⟩ unconstrained tension the reduction was only 0.1% (with c_{33} correspondingly reduced from 0.18 to 0.17). For biaxial tension and plane strain the reduction was about 8%, and the corresponding value of c_{11} ($= c_{22}$) was reduced from 0.16 to 0.10. The same analysis was also extended to the case of {110} ⟨1$\bar{1}$0⟩ simple shear, and predicted an ideal strength of 0.5% less than the maximum value of σ_{31}, with a corresponding reduction in the accompanying shear strain c_{31} from 0.30 to 0.28.

It is, therefore, apparent that less error is introduced by equating the maximum stress with the ideal strength in the case of sodium chloride than in the case of argon.

3.5. The Temperature Dependence of the Ideal Strength

It has already been pointed out that: (i) the potential models used in the present calculations ignore the contribution of the kinetic energy of the atoms to the total energy of the system; (ii) the summation procedures used assume each atom to be at its equilibrium bulk lattice site, and thus ignore surface effects, lattice vacancies and thermal displacements. These potential models and summation methods should, therefore, only be used to calculate the ideal strength at 0° K, if the greatest accuracy is to be obtained. Also, for consistency the adjustable parameters in the potential model should be calculated from experimental data appropriate to 0° K. This was done for the model of argon discussed above, but was not possible in the case of sodium chloride, as the van der Waals interaction parameters in the Born-Mayer model have only been determined for room temperature. Most of the other calculations reviewed in the preceding pages also make use of data appropriate to room temperature.

Temperature thus enters into calculations of the ideal strength in terms of its effect on the adjustable parameters in the potential models, and in terms of the effect of the thermal displacements of the atoms on the lattice sums involved. Since similar lattice sums are also involved in the calculation of the adjustable parameters, these two effects are interrelated.

The only treatment of the effect of thermal vibrations on the ideal strength known to this author is an approximate analysis by Zwicky [50]. This indicates a reduction in the maximum $\langle 100 \rangle$ uniaxial tensile stress proportional to the root mean square amplitude of the atomic vibrations. However, some idea of the effect of temperature on $\sigma_{\max}$ can be obtained from the Orowan-Polanyi equation (1), simply by inserting values of the elastic constant, surface energy and interplanar spacing appropriate to different temperatures. Table II lists values of $\sigma_{\max}$ obtained by Kelly [3] in this way for copper, tungsten and α-iron at 0 and 293° K. These results show that $\sigma_{\max}$ is reduced by $\sim 30\%$ over this temperature interval. However, due to the uncertainties in the surface energy values, this estimate may be in error.

There is also a second effect of temperature on the ideal strength. At any temperature above 0° K there is a finite probability of the thermal nucleation of a tiny crack or dislocation loop in the material. In a highly stressed material such an occurrence would inevitably cause fracture. Kelly [3] has considered the probability of the nucleation of a dislocation loop at the surface of a crystal subjected to shear. He concluded that for any material, if only total dislocations were to be nucleated, then the ideal shear strength would show little temperature dependence due to this effect. Kelly also calculated that for copper, if partial dislocations were to be nucleated, then the ideal shear strength might be halved over the temperature interval 300 to 1173° K. Again it is difficult to assess the accuracy of these results, since both the line energy of the dislocation and the stacking fault energy, which were treated as constants in the calculation, in fact vary with both strain and temperature in some unknown manner.

Accordingly, it has to be concluded that no accurate estimates of the temperature dependence of the ideal strength have yet been made.

4. Comparison of Calculated and Experimental Results

Despite the limitations of the ideal strength calculations and the paucity of consistent high strength experimental data, it is interesting to make such comparisons as are possible.

Inthe absence of experimental data on the strength of anything but highly imperfect polycrystalline specimens of argon [54-56], the most meaningful comparisons are for the case of sodium chloride. In this material the highest $\langle 100 \rangle$ tensile strength measured experimentally is 1.08×10^{10} dynes/cm^2 [57]. In comparison, the most accurate calculations estimate the corresponding ideal strength as about 2.5×10^{10} dynes/cm^2, and the Orowan-Polanyi equation gives a value of 4.3×10^{10} dynes/cm^2. It is, therefore, apparent that the gap between theory and experiment is largely closed in this case, but that the ideal $\langle 100 \rangle$ tensile strength has probably still not quite been realised experimentally.

In the case of $\langle 100 \rangle$ uniaxial extension of argon, the most accurate calculations gave

$\sigma_{\max} = 3.45 \times 10^9$ dynes/cm^2. Taking Young's modulus as 4.5×10^{10} dynes/cm^2 (from the experimental data in table V), the surface energy as 35 ergs/cm^2 (the surface tension of liquid argon at the triple point [58]), and the interplanar spacing as 2.65×10^{-8} cm [49], the Orowan-Polanyi equation (1) gives $\sigma_{\max}$ as 7.6×10^9 dynes/cm^2 ($0.17E$).

Thus, in both cases the Orowan-Polanyi equation overestimates $\sigma_{\max}$ by about 2 × as compared to the most accurate calculations. If this is generally true then the gap between theory and experiment has been removed in the case of the very highest tensile strengths observed in silica glass (table I), and reduced to a factor ~ 2 × or less for many other materials.

In the case of iron the reverse situation arises. The highest tensile strength obtained experimentally is 1.31×10^{11} dynes/cm^2 at a strain of 0.049 from a whisker of $\langle 1\,1\,1 \rangle$ orientation [59]. This is higher than the calculated ideal $\langle 1\,0\,0 \rangle$ uniaxial tensile strengths of 1.7×10^9 dynes/cm^2 and 8.90×10^{10} dynes/cm^2 obtained by Milstein [27] for bcc and bct forms of iron respectively. This discrepancy is almost certainly due to the inadequacy of the central-force two-body Morse potential as a model of the bonding in iron.

In the case of the shear calculations, the values of $\tau_{\max}/G$ from the simple Frenkel calculation, from Kelly's extension of Mackenzie's calculation, and from the most accurate sodium chloride calculations, are all in general agreement. The argon calculations and, more particularly, Mackenzie's calculations for the shear of fcc or cph metals on close packed planes give rather lower values of $\tau_{\max}/G$.

Comparison of these results with experiment is complicated by the fact that the calculations were performed for simple shear, while experimental high strengths are almost invariably measured in bending or tension. Consequently, in the experiments there are both shear and tensile stresses acting on any slip system in general. The ideal shear strength under such conditions will probably be less than that for simple shear.

In spite of this, the highest shear strengths observed by Brenner [59] (table I) in the strongest of his copper and silver whiskers are in good agreement with Mackenzie's calculations. The shear strengths observed consistently by Crump and Mitchell [11] (table I) on some slip systems in cadmium whiskers were even higher. Thus, again it would seem that in these instances the gap between theory and experiment is closed, and that these latter values in particular probably do represent experimental realisation of the ideal strength under the particular test conditions involved. In other cases, e.g. Brenner's strongest whisker of iron, the gap between theory and experiment is closed to within a factor ~ 2 ×.

If these conclusions are correct, it follows that the surface is certainly not very much weaker than the interior of the solid.

Since this article was written calculations of the ideal strength of sodium have been published (Z. S. Basinki *et al*, Proc. 2nd Int. Conf. on the Strength of Metals and alloys, Asilomar, 1970, (American Society for Metals, Cleveland, 1971) 118), together with the results of a further determination of the elastic constants of argon (B. Dorner and H. Egger, *Phys. Stat. Sol.* (b) **43** (1971) 611).

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