TENSILE STRENGTHS OF PERFECT CRYSTALS: ANISOTROPY AND EFFECT OF INTERATOMIC POTENTIAL

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ABSTRACT — Computer calculations of various properties related to the behaviour of perfect crystals at high strains were undertaken using a pairwise potential approach. Three tensile deformation modes were considered, two of uniform deformation (constrained and unconstrained) and one of localized deformation, and the effect of the orientation of the tensile axis was studied. The emphasis was put on the maximum stress that can be supported in each deformation mode.

The potentials used were of the Mye type with three combinations of the exponents in the attractive and repulsive terms. In this way conclusions were drawn on the effect of potential ranges on the anisotropy of the elastic constants and maximum stresses, in each deformation mode. The anisotropy is found to increase as the ranges increase, in contrast with the effect on the anisotropy of surface energy.

Correlations between tensile properties and between these and surface energy were investigated and their accuracy assessed.

1 – INTRODUCTION

The subject of the ideal strength of crystals was recently reviewed by Macmillan [1]. In the calculations of the ideal strength, the atoms are assumed to interact by a pairwise central potential and the energy of the crystal is calculated as a function of the imposed strain: the maximum (or ideal) strength is simply related to the slope of the energy curve at the inflection point. Ideal strengths of simple crystals in uniform tension and in uniform shear have been calculated by this method for various directions of the applied stress, both for constrained and unconstrained deformation, e. g. [2-6], leading to values that are in all cases of the order of 0.1M, M being the relevant elastic modulus.

Calculations of ideal stresses for non-uniform deformation have not been attempted in these studies, although they would be relevant to the understanding of fracture by the usual mechanism of crack propagation. Attemps at computer modelling of cracks have nevertheless been made recently, e. g. [7, 8], based on a lattice dynamics approach.

In this paper we report on results of computer calculations of ideal strengths in tension under various regimes. Results were obtained for several orientations of the tensile axis, allowing a detailed study of the anisotropy of the ideal strength. Three Mye type potentials have been used, with the purpose of studying the effect of the potential range on the ideal strength and on its anisotropy.

In uniform constrained tension no transversal relaxation of the atomic positions is allowed, implying that stresses must be applied in transversal directions. In the unconstrained mode of uniform deformation, the equilibrium positions of the atoms in each plane perpendicular to the applied tension are calculated; the crystal is now stress-free transversally. Calculations of this type were only undertaken for tension applied along symmetry axes.

The special, simple mode of non-uniform deformation that is analysed in this work is such that the interplanar distances remain unaltered except for a pair of planes perpendicular to the tensile axis.

All calculations were made for a f. c. c. monoatomic crystal using three Mye potentials, with exponents $6 \mid 9$, $6 \mid 12$ (Lennard-Jones) and $9 \mid 12$. The stored elastic energy for each potential and each deformation mode is found by calculating the appropriate lattice sums which will be derived in the paper. Equations that enable the calculation of the rests of the lattice sums were also derived with which we were able to avoid the necessity, common to all previous calculations, of considering a crystal of finite arbitrary dimensions. The results obtained for the $6 \mid 12$ potential are compared with those available in the literature [1, 5].

For each deformation mode and each potential we calculate the maximum tensile stress $\sigma_{\max}$, the elastic energy stored at maximum stress and Young's modulus, Y, for various directions of tension. A correlation between these properties and also a correlation with the surface energies, γ, previously determined [9], was attempted. In particular, we calculate the values of α_0 in the equation, e. g. [1, 10, 11],

$$\sigma_{\max} = \alpha_0 \left(Y \gamma / r_0 \right)^{1/2} \tag{1}$$

where r_0 is the interatomic spacing in the crystal (1).

In unconstrained uniform deformation it may happen that the crystal reaches a state of unstable equilibrium before the maximum stress is reached. The problem of stability under load was first discussed by Born ([12]; see other references to Born's work in ref. [13]) and is reviewed in refs. [1] and [13]. The difficulty with Born's stability criterion is that it is not coordinate independent, as first pointed out by Hill [14]. Furthermore, the criterion defines stability with respect to a homogeneous perturbation and not with respect to a general perturbation. At any rate, the stress at the onset of instability is an alternative and in principle more correct definition of the ideal stress. But several ideal stresses can then be defined. Various papers on the problem of stability under load have been published in recent years, particularly by Hill and by Milstein; they are reviewed in ref. [13]. A remarkable finding in these studies [15, 6, 13] is that a deformation path under load may bifurcate leading to different crystal structures. These stress-free structures are reached along paths that go beyond the maximum stress.

Considering the difficulties in assessing stability under load, we identify, in this paper, the ideal strength with the maximum stress attained under unconstrained deformation. This is equivalent to assume that all deformation states up to the one at maximum stress are stable. Consequently, we shall not attempt to address the problem of crystal structure transformations induced by stress or strain.

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(1) In the original form of eq. 1 (see ref. 1), r_0 is the interplanar spacing of planes perpendicular to the tensile axis. However, as will be shown, nearly constant values of α_0 in eq (1) are obtained only if r_0 is the interatomic spacing (or proportional to it).

2 – UNIFORM DEFORMATION

Consider a crystal with an atom per lattice point, in which the lattice planes $(p_1\, p_2\, p_3) = (p)$ are at a variable but uniform spacing, equal to $\mu\, d_0\, (\mu \geqslant 1)$, d_0 being the spacing in the unstressed crystal (Fig. 1). In the unconstrained mode of deformation, the atoms in each plane (p) relax to new equilibrium positions which can be calculated by minimizing the energy of the crystal, for fixed μ. The nominal strain is $(\mu - 1)$. A general method to find the minimum energy configuration for each strain is as follows.

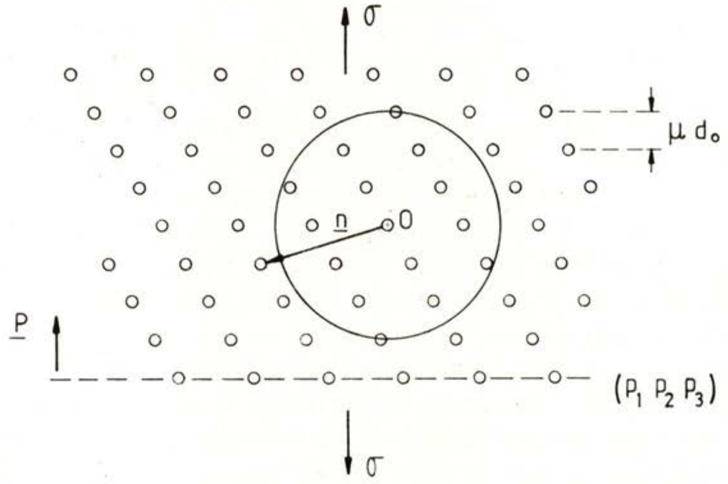

Fig. 1 — A crystal under uniform deformation in tension. The direction of tension is perpendicular to the lattice planes $(p_1\, p_2\, p_3)$. The interplanar spacing of these planes is $\mu\, d_0$, d_0 being the unstrained value.

We take a vector basis in the crystal lattice, $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ (not necessarily a primitive basis), in relation to which we define the Miller indices (p). The unit vector perpendicular to (p) is denoted by $\mathbf{P}$.

Let $\mathbf{t}_3$ be a vector between adjacent unstrained planes (p) and perpendicular to them

$$\mathbf{t}_3 = d_0\ \mathbf{P} \tag{2}$$

and $\mathbf{t}_1$, $\mathbf{t}_2$ two vectors in the plane (p) defining a convenient basis (not necessarily primitive) for the planar lattice in (p). The set $\mathbf{t}_i$ is related to the $\mathbf{e}_i$ by a matrix T

$$[\,\mathbf{t}_1\,\mathbf{t}_2\,\mathbf{t}_3\,] = [\,\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3\,]\ \mathrm{T} \tag{3}$$

or, in a more condensed notation,

$$[\,\mathbf{t}\,] = [\,\mathbf{e}\,]\ \mathrm{T} \tag{4}$$

where $[\,\mathbf{e}\,] = [\,\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3\,]$, for example, is to be regarded as a row matrix. When the crystal is stretched, $\mathbf{t}_3$ changes to

$$\mathbf{t}'_3 = \mu\,\mathbf{t}_3 \tag{5}$$

and $\mathbf{t}_1$, $\mathbf{t}_2$ are transformed into $\mathbf{t}'_1$, $\mathbf{t}'_2$:

$$[\,\mathbf{t}'_1\,\mathbf{t}'_2\,] = [\,\mathbf{t}_1\,\mathbf{t}_2\,] \begin{bmatrix} \alpha_1 & \alpha_3 \\ 0 & \alpha_2 \end{bmatrix} \tag{6}$$

We can always take a non-diagonal element of this transformation matrix as zero, without loss of generality. The atomic positions in the planes of the strained crystal are given by linear combinations of $\mathbf{t}'_1$, $\mathbf{t}'_2$ with the same coefficients that define, in terms of $\mathbf{t}_1$, $\mathbf{t}_2$, the positions in the unstrained crystal. In the constrained deformation mode the matrix in eq. 6 is the identity matrix.

The two sets $\mathbf{t}'_i$ and $\mathbf{t}_i$ $(\mathrm{i} = 1, 2, 3)$ are then related by a matrix D such that

$$[\,\mathbf{t}'\,] = [\,\mathbf{t}\,]\ \mathrm{D}\ ; \quad \mathrm{D} = \begin{bmatrix} \alpha_1 & \alpha_3 & 0 \\ 0 & \alpha_2 & 0 \\ 0 & 0 & \mu \end{bmatrix} \tag{7}$$

The general form of a vector $\mathbf{n}$ between two atoms is

$$\mathbf{n} = \sum_i n_i\ \mathbf{e}_i = [\,\mathbf{e}\,]\ (\,n\,) \tag{8}$$

where $(\,n\,)$ denotes a column matrix with elements n_i. The n_i satisfy certain selection rules, dependent on the crystal structure and vector basis $\mathbf{e}_i$ chosen. For example, if the $\mathbf{e}_i$ are a lattice basis, the n_i are any integers. Eq. 8 can be written as

$$\mathbf{n} = [\mathbf{t}]\ T^{-1}\ (n) \tag{9}$$

When the crystal is deformed, this vector changes to $\mathbf{n}^*$ given by

$$\mathbf{n}^* = [\mathbf{t}']\, T^{-1}\ (n) = [\mathbf{e}]\, TDT^{-1}\ (n) \tag{10}$$

Consider an arbitrary atom for origin. The other atoms are at distances ρ, which, in the deformed crystal, are the moduli of the $\mathbf{n}^*$ vectors. If we denote by $\varepsilon(\rho)$ the pairwise potential, the potential energy per atom, in the field of all other atoms in the deformed crystal, is given by

$$E(\mu;\ \alpha_1, \alpha_2, \alpha_3) = \sum_{\mathbf{n} \neq 0} \varepsilon(n^*) \tag{11}$$

with $\mathbf{n}^*$ given by eq. 10. The sum is for all values of $\mathbf{n} \neq 0$. In the unstrained crystal $-E = 2\,\varepsilon_c$, where ε_c is the cohesive energy per atom. For each μ, the lattice sum (11) is minimized in relation to the α_i. We denote this energy by $\bar{E}(\mu)$ and the volume per atom by v. The applied (nominal) tensile stress, σ, for each μ, is then obtained from

$$\sigma = (1/v)\ d\bar{E}/d\mu \tag{12}$$

because the strain increment is $d\mu$.

Young's modulus, Y_u, can be determined from the slope of $\sigma(\mu)$ as $\mu \to 0$. However it is easier and more accurate to obtain the modulus from the elastic constants (see section 4).

When the deformation is constrained, the vectors $\mathbf{n}^*$ are simply related to μ through

$$\mathbf{n}^* = \mathbf{n} + (\mu - 1)\ (\mathbf{n} \cdot \mathbf{P})\ \mathbf{P} \tag{13}$$

and the elastic energy is obtained from eq. 11. In this case, Young's modulus Y_c was calculated directly for each direction $\mathbf{P}$ by the following method. Since

$$Y_c = (1/v)\ \left(d^2E(\mu)\ /\ d\mu^2\right)_{\mu=0} \tag{14}$$

and noting that (eq. 13)

$$dn^{*2} / d\mu = 2\,(\mathbf{n}\cdot\mathbf{P})\;(\mathbf{n}^{*}\cdot\mathbf{P}) \tag{15}$$

we find upon simple calculations

$$Y_c = \frac{2}{v}\left\{ \sum_{\mathbf{n}.\mathbf{P}>0} (\mathbf{n}\cdot\mathbf{P})^2\, \varepsilon'(n) + 2 \sum_{\mathbf{n}.\mathbf{P}>0} (\mathbf{n}\cdot\mathbf{P})^4\, \varepsilon''(n) \right\} \tag{16}$$

where ε' and ε'' denote derivatives of $\varepsilon(\rho)$ with respect to ρ^2, and the sums are for all $\mathbf{n}$ such that $(\mathbf{n}\cdot\mathbf{P}) > 0$. From the values of Y_c determined in this way for a number of tensile directions it is possible to obtain the elastic constants of the crystal, as we exemplify in section 4. From the elastic constants we then calculate the unconstrained moduli.

3 – LOCALIZED DEFORMATION

Suppose that the distance between two, and only two, crystal planes (p) is changed from d_0 to $d_0 + \delta$ as shown in Fig. 2. The displacement is $\delta\,\mathbf{P}$. The strain will be defined as δ / r_0

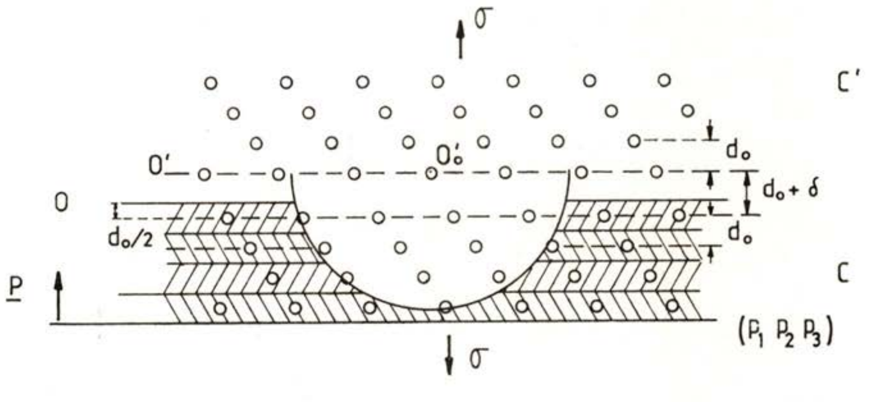

Fig. 2 — A crystal under localized deformation in tension. The direction of tension is perpendicular to the lattice planes $(p_1\,p_2\,p_3)$. The interplanar spacing between a pair of these planes is $d_0 + \delta$, while the other planes remain at the unstrained spacing d_0.

where r_0 is the interatomic spacing (¹). The two half-crystals C and C′ limited by these two planes are rigid. Let $E^*(\delta)$ be the interaction energy between C and C′ per unit area in the plane (p), as a function of δ. The applied stress is

$$\sigma = d\,E^*(\delta) / d\,\delta \tag{17}$$

The potential energy $E^*(\delta)$ is easily derived from the well-known equation [e. g. 9] for the potential energy of interaction, $E^*(0)$, of two half-crystals separated by a plane **P** through an unstrained crystal $(\delta = 0)$:

$$E^*(0) = \frac{1}{V} \sum_{n} (\mathbf{n} \cdot \mathbf{P})\ \varepsilon(n)\ ; \quad \mathbf{n} \cdot \mathbf{P} > 0 \tag{18}$$

where the sum is for $\mathbf{n} \cdot \mathbf{P} > 0$. The quantity $(\mathbf{n} \cdot \mathbf{P})$ is proportional to the number of pairs of interacting planes at a given spacing and is unaltered when the two half-crystals suffer a relative translation $\delta\,\mathbf{P}$, in which case $\mathbf{n}$ in $\varepsilon(n)$ changes to

$$\mathbf{n}' = \mathbf{n} + \delta\,\mathbf{P} \tag{19}$$

Therefore

$$E^*(\delta) = \frac{1}{V} \sum_{n} (\mathbf{n} \cdot \mathbf{P})\ \varepsilon(n')\ ; \quad \mathbf{n} \cdot \mathbf{P} > 0 \tag{20}$$

Young's modulus is defined as the stress increment for a unit increment of the strain δ / r_0 as $\delta \to 0$. Therefore

$$Y_1 = r_0 \left(\frac{d^2 E^*(\delta)}{d\,\delta^2} \right)_{\delta = 0} \tag{21}$$

Using a procedure similar to that described in the derivation of eq. 16 we find

$$Y_1 = 2 \frac{r_0}{V} \left[\sum_{n} (\mathbf{n} \cdot \mathbf{P})\ \varepsilon'(n') + 2 \sum_{n} (\mathbf{n} \cdot \mathbf{P})^3\ \varepsilon''(n') \right] \tag{22}$$

where the sums are, again, for all $\mathbf{n}$ such that $\mathbf{n} \cdot \mathbf{P} > 0$.

(¹) The strain has to be defined in relation to a reference length in the crystal, the same for all orientations of the tensile axis. It is misleading to define strain in relation to the interplanar spacing d_0.

4 – APPLICATION TO F.C.C. CRYSTALS, MYE POTENTIALS

The general equations derived above were applied to f.c.c. crystals in which the atoms interact by a Mye potential with exponents e, e′:

$$\varepsilon(\rho) = \varepsilon_0 \left[(\sigma/\rho)^{e'} - (\sigma/\rho)^{e} \right], \quad e' > e \tag{23}$$

In this equation ε_0 and σ are constants that can be related to the cohesive energy ε_c and to the interatomic distance r_0 in the crystal (see ref. 9). The values of e, e′ used were combinations of 6, 9 and 12. A quantity of interest is the second derivative of $\varepsilon(\rho)$ at the minimum, which is a measure of the elastic stiffness of the bond between a pair of atoms. These values and other relevant parameters of each potential (taken from ref. 9) are included in Table 1.

TABLE 1 — Various parameters of the Mye potentials used

	6 | 9 Potential	6 | 12 Potential	9 | 12 Potential
σ / r_0	0.91710	0.91729	0.91747
$\varepsilon_0 / \varepsilon_c$	0.69769	0.46456	1.39026
$(d^2\varepsilon / d\rho^2)$ *	5.0646	7.8880	15.5292

* Second derivative at the minimum $\varepsilon(\rho)$ in ε_c units.

With unit vectors, $\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3$, parallel to the cube axes, the form of $\mathbf{n}$ is

$$\mathbf{n} = (a/2) \sum_i n_i\, \mathbf{e}_i \tag{24}$$

where a is the lattice parameter (cube edge, $a = \sqrt{2}\, r_0$) and the n_i are integers such that

$$\sum_i n_i = \text{even integer} \tag{25}$$

In the following equation, $\mathbf{n}$ and n are expressed in $a/2$ units.

The lattice sums that intervene in the calculation of the energy in the three deformation modes are of the following types.

To obtain the energy in uniform deformation, it is necessary to calculate series of the type

$$S_e = \sum_{\mathbf{n} \neq 0} \left(\frac{1}{n^*} \right)^e \tag{26}$$

where $\mathbf{n}^*$ is related to $\mathbf{n}$ by eqs. 10 and 13, respectively for the unconstrained and constrained deformation modes.

In the localized deformation mode the lattice sums for the energy are of the form

$$C_e(\delta) = \sum_{\mathbf{n}} \frac{\mathbf{n} \cdot \mathbf{P}}{(n')^e} \tag{27}$$

where $\mathbf{n}'$ is defined by eq. 19 and the sum is for all $\mathbf{n}$ such that $\mathbf{n} \cdot \mathbf{P} > 0$.

Finally the sums that enter in Young's moduli (eqs. 16 and 22) are of the types

$$\sum (\mathbf{n} \cdot \mathbf{P})^\alpha \, n^{-(e+\alpha)} \text{ and } \sum (\mathbf{n} \cdot \mathbf{P})^{\alpha-1} \, n^{-(e+\alpha)} \, ; \; \alpha = 2{,}4 \tag{28}$$

summed for all $\mathbf{n}$ such that $\mathbf{n} \cdot \mathbf{P} > 0$. As already pointed out, in eqs. 26-28, $\mathbf{n}$ is expressed in $a/2$ units, so that the components n_i are integers satisfying eq. 25.

The sums S_e and C_e were calculated with great precision. A direct sum was obtained up to a chosen value of n; the rest of the sum was obtained by replacing the corresponding part of the crystal by a continuum. The appropriate equations are derived in the Appendix.

The sums (28) for Young's moduli were calculated by direct sum up to $n = 10$ (in $a/2$ units). The maximum error in such truncated sums, estimated from values obtained for $n = 15$, is 1 %.

Calculations in the unconstrained mode were done exclusively for the tensile axis parallel to [002] and [111] directions. The method developed in section 2 was used to find the relaxed configuration which, in both cases, depends on one parameter only (1).

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(1) This restriction to one parameter calculations is a constant in the literature. The method outlined in section 2 can, of course, be used to extend the calculations to other directions of tension.

The vectors $\mathbf{t}_1, \mathbf{t}_2$ in the plane perpendicular to the tensile axis were chosen parallel to $<110>$, both for [002] and [111] tension, as shown in Fig. 3. The matrix D (eq. 7) then has $\alpha_3 = 0$ and $\alpha_1 = \alpha_2 = \alpha$.

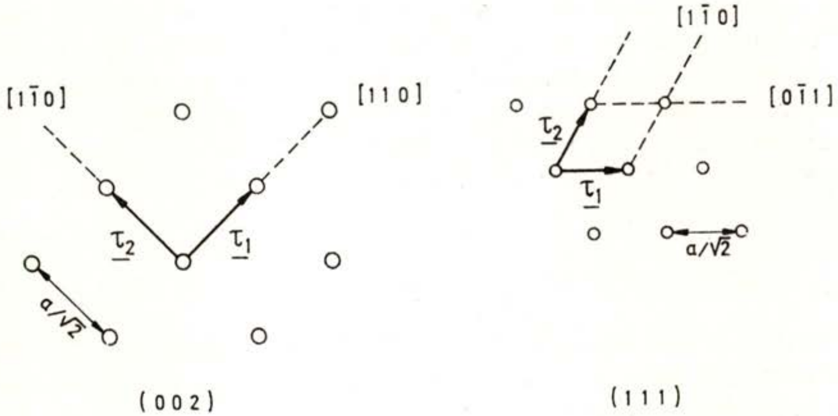

Fig. 3 — Choice of vector bases in (002) and (111) planes.

The elastic moduli in uniform deformation can be expressed in terms of the elastic constants. In the unconstrained mode, the modulus for tension in the direction $[\,p_1\, p_2\, p_3\,]$ is easily found to be

$$Y_u^{-1} = (1/p^4)\ [A\ s_{11} + B\,(2\ s_{12} + s_{44})] \tag{29a}$$

where

$$\begin{aligned} A &= p_1^4 + p_2^4 + p_3^4 \\ B &= p_1^2\ p_2^2 + p_2^2\ p_3^2 + p_3^2\ p_1^2 \end{aligned} \tag{29b}$$

and the s_{ij} are the elastic compliances. It is also easy to obtain equations for the Poisson ratio corresponding to [002] and [111] tension. In the constrained mode of deformation, the modulus is given by

$$Y_c = (1/p^4)\,[A\,c_{11} + B\,(2\,c_{12} + 4\,c_{44})] \tag{30}$$

where the c_{ij} are the stiffnesses, related to the s_{ij} by well-known equations [e. g. 16]. It is then possible, by calculating the constrained moduli for a few directions, to obtain all the c_{ij}, making use of Cauchy's relation $c_{44} = c_{12}$. The s_{ij} are then calculated and, from them, the unconstrained moduli can be determined for the various directions of tension.

In unconstrained deformation, the stress obtained from eq. 12 is a nominal stress (force divided by the initial area). The true stress can easily be found from the values of α in the equilibrium configurations; it is obtained by multiplication of the nominal stress by α^{-2}. Finally, it is possible to obtain the transversal stress in constrained tension parallel to [002] and [111]. The transversal stress is a negative two-dimensional pressure p, which, for each μ is given by

$$p = 1/(\mu d_0) \cdot dE(\mu, \alpha)/dS = 1/(\sqrt{2}\,\mu) \cdot dE/d\alpha \qquad (31)$$

where S is the area per atom in the plane perpendicular to the tensile axis ($S_{002} = 1/2\ \alpha^2 a^2$; $S_{111} = \sqrt{3}/4\ \alpha^2 a^2$). The derivative is taken for $\alpha = 1$.

5 — RESULTS AND DISCUSSION

All quantities will be expressed by taking ε_c (the cohesive energy per atom) and r_0 (the interatomic spacing in the crystal) as units. For example, elastic stiffnesses and Young's moduli will be expressed in ε_c / r_0^3 units.

Table 2 gives the values of the elastic constants c_{ij} and s_{ij} for each potential. The anisotropy ratio is also included. The anisotropy increases as the exponents in the potential decrease (increasing range). The elastic stiffnesses increase as the curvature of the potential at the minimum increases (cf. values in Table 1).

TABLE 2 — Elastic constants *

Potential	c_{11}	$c_{12} = c_{44}$	s_{11}	s_{12}	s_{44}	$2c_{44}/(c_{11}-c_{12})$
6 | 9	23.21	13.88	0.0780	-0.0292	0.0720	2.977
6 | 12	31.69	18.12	0.0540	-0.0197	0.0552	2.672
9 | 12	48.62	26.60	0.0335	-0.0119	0.0376	2.415

* c_{ij} in ε_c / r_0^3 units for each potential; s_{ij} in $r_0^3 /\ _c$ units.

However, a simple correlation between the c_{ij} and the curvature cannot be established. This is not surprising considering that the equilibrium distance in the crystal is always smaller than the equilibrium distance of a pair of atoms [9].

Fig. 4 shows the energy curves for constrained tension in the [111] direction for the three potentials. The location of the inflection points is indicated. In Fig. 5 are shown the stress-strain curves corresponding to Fig. 4. Similar curves are obtained for other directions and for other deformation modes.

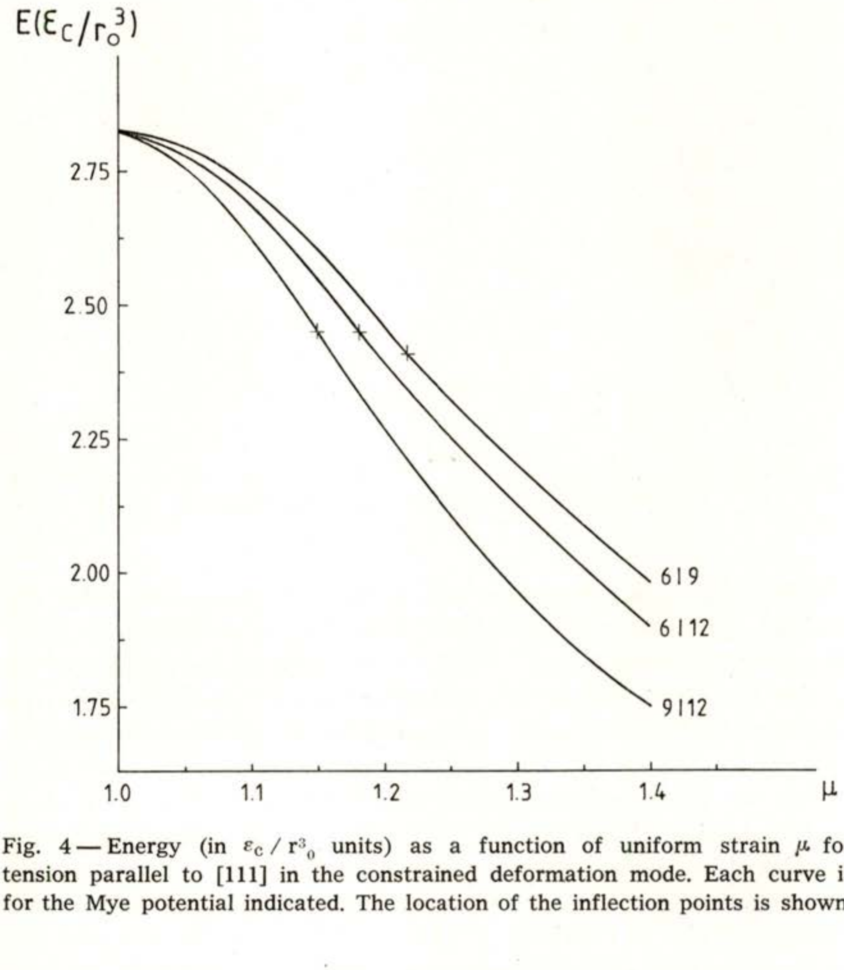

Fig. 4 — Energy (in ε_c / r^3_0 units) as a function of uniform strain μ for tension parallel to [111] in the constrained deformation mode. Each curve is for the Mye potential indicated. The location of the inflection points is shown.

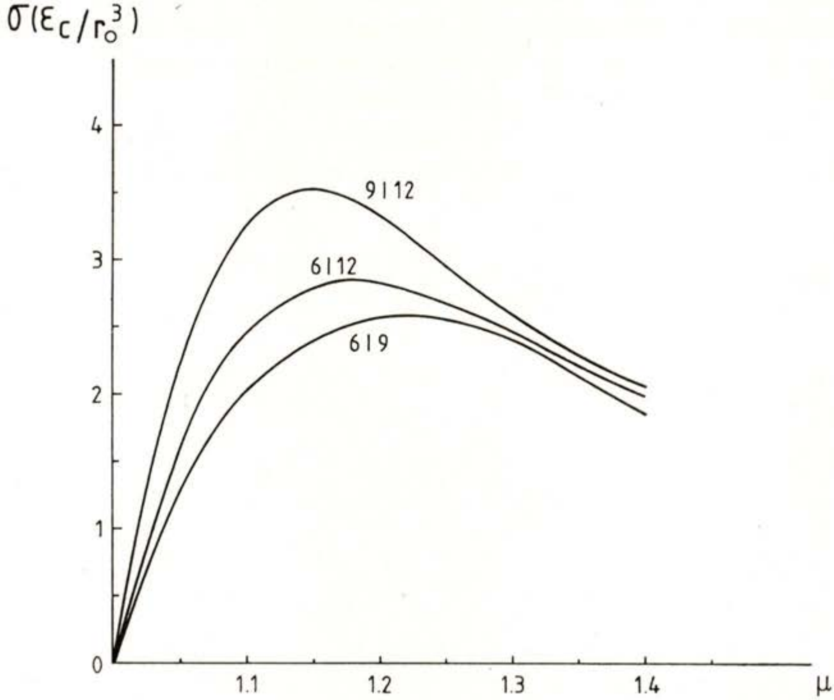

Fig. 5 — Nominal stress-strain curve for [111] uniform constrained tension. Each curve is for the Mye potential indicated.

In Table 3 are indicated the values of Young's modulus for various orientations of the tensile axis in each deformation mode. As already explained, the moduli for the constrained and localized modes were determined directly from eqs. 15 and 22, while the unconstrained moduli were calculated from the elastic constants. The values included in Table 3 for the constrained and localized modes are for tensile directions perpendicular to the more close packed lattice planes up to (135). Many other directions were calculated but in Table 3 we include only one more, for [1 15 19] tensile axis. The ratio of the moduli for [111] and [002] is also shown in Table 3, confirming that the anisotropy increases as the range of the potential increases. It is remarkable that the anisotropy of surface energy (and also of evaporation energy) varies in the opposite way with the range of the potentials [9]. It is also noticeable that the unconstrained moduli are only slightly smaller

TABLE 3 — Young's moduli (c / r_0^3 units) and Poisson ratios

Constrained; Localized

Tensile axis	6 | 9 Potential		6 | 12 Potential		9 | 12 Potential	
	constrained	localized	constrained	localized	constrained	localized
111	35.50	23.81	46.81	30.33	69.40	43.37
002	23.21	19.58	31.69	25.24	48.62	36.57
022	32.43	21.15	43.03	27.20	64.20	39.31
113	29.00	20.68	36.81	26.61	58.41	38.48
133	33.32	21.89	44.13	28.08	65.71	40.45
024	29.11	20.23	38.94	26.12	58.59	37.88
224	32.43	21.95	43.03	28.15	64.20	40.53
115	25.79	19.90	34.86	25.66	52.98	37.17
135	31.01	20.91	41.28	26.93	61.80	38.96
1 15 19	31.97	20.98	42.46	27.01	69.39	39.08
Ratio extreme values	1.53	1.22	1.48	1.20	1.43	1.19

Unconstrained (Values in brackets are calculated Poission's ratios).

Tensile axis	6 | 9 Potential	6 | 12 Potential	9 | 12 Potential
111	32.75 (0.179)	42.93 (0.185)	63.32 (0.190)
002	12.82 (0.374)	18.52 (0.364)	29.85 (0.354)
Ratio extreme values	2.56	2.32	2.12

than the constrained ones for [111], but appreciably smaller for [002]. This is related to the small relaxation associated with tension along [111], reflected in the small value of the Poisson ratio, also listed in Table 3. In all modes, the extreme moduli are for [111] (maximum) and [002] (minimum). It is also noted that Poisson's ratio increases with the range of the potential for [002] tension but decreases with the range for [111] tension. The behaviour in unconstrained tension was found to be anomalous at high strains in the sense that the transversal dimensions go through a minimum and then increase as the tensile strain increases. This result was previously reported in ref. [5].

The maximum stresses are indicated in Table 4 for various orientations of the tensile axis in each deformation mode studied. The largest maximum stress is in all cases for [111] tension while the smallest value was obtained for [0 30 38] among the directions investigated. The maximum stress is larger in the unconstrained mode than in the constrained one, but the difference is small. The maximum stress in localized deformation is appreciably smaller than in uniform deformation, by a factor that varies between 1.40 and 1.95. This factor increases from the $6 | 9$ to the $9 | 12$ potential.

The transversal tension, p, at maximum stress in constrained deformation was calculated from eq. 31. The values of p are about 9 % and 31 % of the maximum stress, respectively for [111] and [002] tension. The lower value for [111] tension is related to the smaller transversal contraction that occurs in this case.

Our results on maximum stresses and Young's moduli for the $6 | 12$ potential were compared with those obtained by Macmillan and Kelly [5] for argon, using the same potential and appropriate values of the potential constants. The agreement is excelent, as we show with the following examples. The ratio of the extreme maximum stresses in constrained tension is $3.42/2.64 = 1.295$ in ref. [5], while our value is $2.856/2.215 = 1.289$. The ratio σ_{max} / Y_c in [002] constrained tension is 0.083 in both calculations. The ratio of maximum true stresses in [002] unconstrained and constrained tension is $3.45/3.17 = 1.088$ in ref. [5] and $2.861/2.645 = 1.082$ in the present work.

Other characteristics of the critical state at maximum stress were determined in the calculations, related to the stored elastic energy and to the deformation at maximum stress. In Table 5 are

TABLE 4 — Maximum stress (ε_c / r_0^3 units)

	6 | 9 Potential		6 | 12 Potential		9 | 12 Potential	
	constrained *unconstrained*	localized	constrained *unconstrained*	localized	constrained *unconstrained*	localized
111	2.582 *2.607 - 2.640* (*a*)	1.461	2.856 *2.882 - 2.922*	1.551	3.539 *3.566 - 3.616*	1.814
002	2.323 *2.388 - 2.548*	1.414	2.645 *2.703 - 2.861*	1.524	3.420 *3.476 - 3.649*	1.815
022	1.944	1.401	2.223	1.499	2.828	1.774
113	2.068	1.411	2.362	1.509	3.024	1.789
133	2.125	1.412	2.403	1.508	3.032	1.779
024	1.950	1.389	2.243	1.492	2.888	1.774
224	2.221	1.417	2.500	1.513	3.157	1.784
115	2.129	1.414	2.458	1.515	3.147	1.801
135	2.008	1.397	2.292	1.496	2.926	1.775
0 30 38	1.935	1.391	2.215	1.493	2.827	1.772
Ratio extreme values	1.33 *1.09*	1.05	1.29 *1.07*	1.04	1.25 *1.03*	1.02

(*a*) First value in italic is nominal stress; second value in italic is true stress.

TABLE 5 — Deformation and stored energy at maximum stress

Constrained

Property	6 | 9 Potential	6 | 12 Potential	9 | 12 Potential
μ	1.21 - 1.28 (1.06)	1.18 - 1.24 (1.05)	1.15 - 1.20 (1.04)
Stored energy (ε_c / r_0^3 units)	0.324 - 0.472 (1.46)	0.321 - 0.465 (1.45)	0.340 - 0.500 (1.47)

Unconstrained

Property	6 | 9 Potential [111] [002]	6 | 12 Potential [111] [002]	9 | 12 Potential [111] [002]
μ	1.207 1.283 (1.063)	1.170 1.257 (1.074)	1.147 1.210 (1.055)
α	0.9937 0.968 (1.026)	0.9932 0.972 (1.022)	0.9930 0.976 (1.017)
Stored energy (ε_c / r_0^3 units)	0.386 0.439 (1.14)	0.353 0.476 (1.35)	0.361 0.494 (1.37)

Localized

Property	6 | 9 Potential	6 | 12 Potential	9 | 12 Potential
δ (r_0 units)	0.18 - 0.24 (1.33)	0.16 - 0.18 (1.13)	0.13 - 0.14 (1.08)
E_{max} (ε_c / r_0^2)	0.197 - 0.262 (1.33)	0.178 - 0.209 (1.17)	0.169 - 0.188 (1.11)

Values in brackets are the ratios of extreme values.

indicated, for each potential and each deformation mode, the ranges of values found for the various tensile directions. The extreme values of the deformation parameter, μ, at maximum stress occur for [111] and [002] tension, respectively for the largest and smaller μ. The values of the stored energy vary only slightly with orientation; the extreme values correspond to tensile directions which depend on the potentital and are not in general low index directions. Neverthless the larger values seem to occur near [024] and the smaller values near [002] in uniform deformation and near [111] in localized deformation. It is also noted that the energy stored at maximum stress is not much different in the two modes of uniform deformation.

The ratio between maximum stress and Young's modulus is listed in Table 6. Nominal stresses were used in the case of unconstrained deformation. There is a fair uniformity in the values, although the ratios for unconstrained deformation in [002] are noticeably larger. In general, then, the maximum stress ranges from Y/5 to Y/23.

TABLE 6 — Ratio between maximum stress and Young's modulus (x 100)

Direction of tension	6 | 9 Potential			6 | 12 Potential			9 | 12 Potential		
	unconst.	const.	local.	unconst.	const.	local.	unconst.	const.	local.
111	8.0	17.3	6.1	6.7	6.1	5.1	5.6	5.1	4.2
002	18.6	10.0	7.2	14.6	8.3	6.0	11.6	7.0	5.0
022		6.0	6.6		5.2	5.5		4.4	4.5
113		7.1	6.8		6.4	5.7		5.2	4.6
133		6.4	6.5		5.4	5.4		4.6	4.4
024		6.7	6.9		5.8	5.7		4.9	4.7
224		6.8	6.5		5.8	5.4		4.9	4.4
115		8.5	7.1		7.0	5.9		5.9	4.8
135		6.5	6.7		5.6	5.6		4.7	4.6

Using the values of (unrelaxed) surface energies calculated in ref. [9] for the same potentials, we determined the values of α_0

defined by eq. (1). The results are as follows. In constrained deformation α_0 increases from the 6 | 9 to the 9 | 12 potential. The extreme values for the 6 | 9 potential are 0.48-0.69; for 6 | 12: 0.51-0.70; and for 9 | 12: 0.57-0.82. The first value corresponds to [022] and the second to [002]. The values for unconstrained deformation (nominal stresses) are as follows (first value for [111], second for [002]): 6 | 9: 0.66-0.95; 6 | 12: 0.67-0.94: 9 | 12: 0.78-1.07.

Finally, the values of α_0 for localized deformation are surprisingly uniform: they range from 0.42 to 0.44 for each of the 6 | 9 and 6 | 12 potentials and from 0.45 to 0.50 for the 9 | 12 potential.

Various correlations involving the energy stored at maximum stress have been attempted. For example, the ratio between the maximum stored energy and the surface energy ranges from 0.41 to 0.53 in localized deformation.

6 – SUMMARY

The calculations described in this paper were aimed at studying the effect of the interatomic potential on various crystal properties with interest for the mechanical behaviour of materials. The tensile properties at low stresses (elastic stiffness) and at maximum stress (ideal strength, stored energy and deformation) were calculated for each Mye potential as a function of the direction of the tensile axis. The anisotropy of these properties was found to increase as the range of the attractive and/or repulsive terms in the potential increases. This is in contrast with the effect of range on the anisotropy of the surface energies. The anisotropy of the maximum stress is fairly small for all potentials, indicating that there is not a well-defined cleavage plane.

The consideration of different tensile modes is another matter of interest in the paper. It was concluded that in the localized deformation mode, the maximum stress is reduced by a factor of 1.5-2 compared to the values in uniform deformation. Finally, correlations between tensile properties and surface energy, such as eq. 1, were analysed and the numerical factors in the correlations were determined.

APPENDIX — CALCULATION OF LATTICE SUMS

The sum S_e defined in eq 26 is calculated term by term for all combinations of integers n_i satisfying eq. 25 and such that

$$n_1^{*2} + n_2^{*2} + n_3^{*2} \leqslant M^2$$

and the corresponding number of terms, or atoms, N, is counted. The vector $\mathbf{n}^*$ is defined by eqs. 10 or 13. The rest of the sum is obtained from an integral over a continuum distribution in the region outside the sphere where the N atoms are located (Fig. 1). Since the volume per atom is $(a^3/4)\, D$, where $D = |\det D|$ is the volume ratio between the strained and unstrained crystal, the radius $R_0\,(a/2)$ of the sphere is given by

$$4\pi R_0^3 / 3 = 2ND$$

The rest of the series, S'_e, is obtained by integration in ρ over the region outside the sphere, where the atomic density is $4\,(a^3 D)^{-1}$:

$$S'_e = (4\pi/2\,D) \int_{R_0}^{\infty} \rho^{2-e}\, d\rho = 2\pi\; R_0^{3-e}\, D^{-1} / (e - 3)$$

The series S_e is then calculated from

$$S_e = \sum_{\rho \leq M} \rho^{-e} + S'_e$$

When the value of M is changed from 10 to 15 the relative changes in the energy values obtained for the 6 | 9 potential are less than 2.10^{-3} %. The accuracy is even better for the other potentials.

The series $C_e\,(\delta)$ defined by eqs. 27 and 19 is calculated term by term for all values of n_i such that

$$n_1'^2 + n_2'^2 + n_3'^2 \leqslant M^2 \;;\quad n'_i = n_i + \delta p_i / p$$

where δ is expressed in a/2 units. The corresponding N atoms are within a hemisphere centred at atom $0'_0$ in the first plane $0'$ of crystal C′ (see Fig. 2). The radius of this hemisphere, R_0 (a/2), is given by (see ref. 9)

$$(2\pi/3)\, R_0^3 - \pi R_0^2 (\delta + 1/p) = 2N$$

Note that $1/p + \delta$ is the interplanar spacing (in a/2 units) across the two half-crystals. Crystal C, outside the hemisphere, is replaced by a continuum distribution of lamella of thickness d_0, centred in each plane, with an atomic density $4/a^3$ (Fig. 2). The procedure is similar to that used for the sums that give the surface energy [9]. The integration region, outside the hemisphere, is the difference between: i) the volume below plane 0′ outside the hemisphere; ii) the volume of a lamella of thickness $d_0/2 + \delta$, adjacent to plane 0′, and outside the hemisphere.

The integrals over these two regions are calculated in spherical coordinates, ρ (in a/2 units), θ and ϕ. But

$$\mathbf{n} \cdot \mathbf{P} = \rho \cos\theta - \delta$$

The integrals that give the rest of sum $C_e(\delta)$ are of the form (upon integration in ϕ)

$$\frac{2\pi}{2} \iint (\rho \cos\theta - \delta)\ \rho^{2-e} \sin\theta \ d\rho \ d\theta$$

where a factor 1/2, corresponding to the atomic density in a/2 units, has been introduced.

The integral over region i) is for ρ between R_0 and ∞ and for θ between 0 and $\pi/2$. The result is

$$C'_e = \frac{\pi}{2(e-4)} \frac{1}{R_0^{e-4}} - \frac{\pi}{e-3} \frac{\delta}{R_0^{e-3}}$$

The integration limits for region ii) are: ρ between R_0 and $(1/p + \delta)/\cos\theta$ and θ between $\cos^{-1}[(1/p + \delta)/R_0]$ and $\pi/2$. The result is

$$C''_e = \frac{\pi}{2p^2} \frac{1}{e-2} (1 - p^2 \delta^2) \frac{1}{R_0^{e-2}}$$

The series C_e is then calculated from

$$C_e(\delta) = \sum_{\rho \leq M} (\mathbf{n} \cdot \mathbf{P}) \, \rho^{-e} + C'_e - C''_e$$

Note that for $\delta = 0$ the result corresponds to that derived in ref. 9 for the sums used in the calculation of surface energies (the series C_e in that paper is related by a factor 2/p to the one being used here).

When M is changed from 10 to 15, the relative change in the interaction energy E(0) obtained by this method for (002), potential 6 | 9, is 6.10^{-3} %. For the other potentials the error is even smaller.

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