A NEW THEORETICAL DETERMINATION OF YIELD STRESS
BASED ON THE CONCEPT OF EFFICIENT AREA OF STRESS

Abstract

This study presents a new theoretical determination of yield stress for pure mono-crystal materials based on the concept of the Efficient Area of Stress (EAS). From the atomic yield stress on the atomic surface a^2, given by the model of Orowan, the macroscopic yield stress is then obtained through a Scale Law of Measure (SLM) which depends only on the lattice spacing and a constant Λ. This relation shows that the efficient atomic dimension is a fractal dimension. The precision obtained by the SLM is of an atomic order compared to the error (10^2 to 10^4 MPa) obtained by classical theories. The SLM gives also new theoretical relations for the elastic limit of strain, the toughness and the fracture strength. The SLM is finally extended to non pure materials to take into account the microstructures (grain size, impurity, phases, solutions, etc.) and the temperature effects by introducing the concept of an "efficient atomic distance".

Key words: *Yield stress, atomic cleavage fracture, scale factor, efficient area of stress, fractal.*

Résumé

Cette étude présente une nouvelle détermination théorique de la limite élastique pour les matériaux mono-cristaux basée sur le concept de Section Efficace de Contrainte. A partir de la limite élastique atomique sur la surface atomique a^2, donnée par le modèle d'Orowan, la limite élastique macroscopique est alors calculée à partir d'une loi de facteur d'échelle (SLM) qui ne dépend que de la dimension atomique a et d'une constante Λ. Cette relation montre que la distance atomique effective est une dimension fractale. La précision obtenue par la SLM est d'ordre atomique en comparaison avec l'erreur (10^2 à 10^4 MPa) obtenue par les théories classiques. La SLM donne aussi de nouvelles relations théoriques pour la limite élastique de déformation, pour la ténacité et pour la limite de rupture. La relation est finalement étendue aux matériaux non purs pour prendre en considération la microstructure (dimension des grains, impuretés, phases, solutions, etc.) et l'effet de température par l'introduction du concept de "distance effective atomique".

Mots clés: *Limite élastique, limite atomique de scission, facteur d'échelle, surface effective de contrainte, fractales.*

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ملخص

يقدم هذا البحث تصميما جديدا نظريا لحد المرونة للمواد الخالصـة إنطلاقا من حد المرونة الذرية على المساحـة الذرية المعطاة من معادلة Orowan. فحد المرونة محسوبة إنطلاقا من قانون السلم الذي لا يتعلق إلا بالمسافة الذرية الفعلية و من ثابتة. هذه العلاقة تبين أن المسافة الـذرية هي مسافة جزئية. الدقة المحصلة عليها هي ذرية مقارنة بالخطئ المحصل عليه من طرف النظريات الكلاسكية. التصميم المقدم يعطي أيضا علاقات نظرية جديدة للتحصل على حد مرونة التشوه، المتانة ، حد الانكسار. الـعلاقة طبقـت أيضـا على المواد الـغير الخالصـة لأخذ بعين الاعتبار التركيبة المجهرية (مسافة الحبيبة ، الشابهات، الطور، المحلول....) وفعل الحرارة بإدخال معنى "المسافة الذرية الفعلية".

الكلمات المفتاحية: حد المرونة، الحد الذري الانشطار، عامل السلم، المسافة الفعلية للضغط، مسافة جزئية.

$\mathbf{S}$ince Orowan, many models have been presented for the theoretical determination of yield stress from the cleavage fracture at the atomic level. The models of Kelly [1] and Macmillan [2], the electrostatic models or the spring model [3] are all based on the original Orowan model, which was first made in 1958 [4]. Theses models depend only on the Young modulus which can be obtained from geometrical values through an analysis of the interatomic energies and force [5]. Nevertheless, none of these models has so far obtained a clear satisfaction since they all give theoretical values, which are 100 to 1000 MPa higher than the experimental values. This error comes from a lack of a renormalisation to take into account the size effect when passing from a microscopic dimension to a macroscopic dimension. Springs, electrostatic or dislocation models must also take into account the complexity of the atomic world: real forces between atoms, number of neighbouring atoms, degree of fill, plans of slip and crystalline defects (micro-cracks, interstices, Frankel and Schottky defects, dislocations, joins at grains, precipitate, etc.). The classic literature gives also the theories of Hall [6] and Petch [7], Stroh [8], Cottrell [9] and Smith's [10], which can give the cleavage fracture, but only at the grain size level.

In this paper a new theoretical determination of yield stress for pure materials is presented. This theory uses the concept of the Efficient Area

of Stress (EAS). The effective stress is only acting on the EAS. Damage is defined by the reduction of the area under stress. This definition was first given by Murakami [11]. The concept of area reduction and EAS has also been successfully used by Hult [12], Chaboche [13] and Krajcinovic [14] to develop their CDM (Continuum Damage Mechanics) theory at the grain scale (10^{-6}). In this study this concept of EAS is extended to the atomic level (10^{-10}) by dividing an apparent microscopic area a^2, represented by the atomic model of Bohr, into a space of matter c^2, called the EAS which sustain stress, and an empty space v^2. From the atomic yield stress on a^2, given by the model of Orowan, the macroscopic yield stress is then obtained through a Scale Law of Measure (SLM) which depends only on the atomic size a and a constant Λ. The possible extension of the SLM to give new relations for the elastic limit of strain, the toughness and the fracture strength is investigated, but future work has to be done to fully investigate these relations.

The concept of SLM is finally extended to poly-crystals to take into account the effects of microstructures and temperature through the introduction of the concept of the "effective atomic dimension" which represents the affected new lattice pacing.

THE CLASSICAL LAWS OF YIELD STRESS AT THE ATOMIC LEVEL FOR PURE MATERIALS

The elastic (cleavage) limit S_{ya} of a pure material at the atomic level depends on the equilibrium distance between atoms r_0. This cleavage fracture is given in the following form:

$$S_{ya}^2 = \xi E \gamma / r_0 \tag{1}$$

The value of ξ is given equal to $2/\pi$ by Kelly [1] and Macmillan [2], 2 by the electrostatic model [3] or 4 by the springs model [3]. These models belong to the original model developed for the first time by Orowan in 1958 [4], which has a value of 1.

The energy of a crystal is equal to the sum of the Coulomb energy of attraction U_a and the potential energy of repulsion U_r [3,5]:

$$U_a = -M\varpi / r \text{ et } U_r = zb_1 / r^{b_2} \tag{2}$$

z is the neighbouring atoms. b_1, b_2 are the constant of repulsion. M is the constant of Madelung. ϖ is the factor of colomb $\varpi = q^2 / (4 \pi \varepsilon_0)$. The total energy is then equal to:

$$U = B_1 / r + B_2 / r^n \tag{3}$$

B_1 and B_2 are constants of energy. The equilibrium interatomic distance is obtained from by letting: $dU/dr = 0$. The force at a distance r is given by:

$$F = dU / dr \tag{4}$$

Stiffness is also given by:

$$K = dF / dr = d^2U / dr^2 \tag{5}$$

For small strain, we have: $K = (d^2U / dr^2)$ at $r = r_0$ which gives [5]:

$$K = M \varpi / r_0^3 \tag{6}$$

Young's modulus is given by [5]:

$$E = K / r_0 = M \varpi / r_0^4 \tag{7}$$

Some values of K and E are shown in table 1.

Bounding	Material	K Nm^{-1}	E GPa
Covalente	C-C	180	1000
Ionique	Na-Cl	9 à 21	30 à 70
Metallic	Cu-Cu	15 à 40	30 à 150
Hydrogen	H_2O-H_2O	2	8

Table 1: Values of K and E.

A NEW THEORETICAL DETERMINATION OF YIELD STRESS FOR PURE MATERIALS

Definitions of the microscopic and the macroscopic EAS

First, we have to define the following four areas:

- A square microscopic apparent area a^2 that represents the atomic section of the material according to the quantum model of Bohr (with actually a difference of $\pi/4$). The elastic limit of this surface is called the microscopic apparent yield S_{ya}.

- The precedent microscopic apparent area is made of two areas: an atomic EAS area c^2 and a void v^2. The elastic limit on c^2 is called the microscopic effective yield S_{yc}.

- A square apparent macroscopic area A^2 of 1 m² composed of $n^2 a^2$. The elastic limit on this surface is called the macroscopic apparent yield S_{yA}.

- The precedent macroscopic apparent area is made of two areas: A macroscopic EAS C^2 composed of $n^2 c^2$ and a macroscopic void V^2. The elastic limit on C^2 is called the macroscopic effective yield S_{yC}.

The scale factor for the four areas is the same:

$$A^2/a^2 = C^2/c^2 = n^2 \tag{8}$$

Proposition 1: Stiffness is independent of scale.
Proposition 2: Toughness is independent of scale.
Proposition 3: the macroscopic and microscopic elastic limits differ only on a geometrical scale factor. This concept is called the "geometrisation" of physics.

In using propositions 1 and 2, one can demonstrate that the effect of scale n [15] is $n^{3/2}$ on critical forces, $n^{1/2}$ on displacements and $n^{-1/2}$ on stresses. This means that:

$$S_{y_2} = S_{y_1} / \sqrt{n} \tag{9}$$

Calculation of stress limits

- **Calculation of microscopic apparent yield S_{ya}**

We take equation (1) of Orowan: $S^2_{ya} = E \gamma / a$. By using [15]: $\gamma = E a / (2\pi)^2$ we find:

$$S_{ya} = E / (2\pi) \tag{10}$$

- **Calculation of macroscopic apparent yield S_{yA}**

Proposition 4: A material is said to be perfect when one supposes that it is filled by the square atoms without letting any emptiness. We have from the definitions of A:

$$A = na = 1$$

then:

$$n = 1 / a \tag{11}$$

By using equation (9) and (10), we obtain:

$$S_{yA} = S_{ya} \sqrt{a} = E / (2\pi) \sqrt{a} \tag{12}$$

- Calculation of microscopic EAS c

Proposition 5: the atomic EAS is defined as a square area c^2 which is the real efficient area that sustains the stress and then gives the real stress in the atomic level.

$$C^2/c^2 = n^2 \ , \quad \text{with} \quad n = 1/a$$

$$S_{yC} = S_{yc}/\sqrt{n}$$

$$S_{yc} = S_{yC}\sqrt{n} = S_{yC}/\sqrt{a} \qquad (13)$$

To find c one can use the scale factor n' between a and c:

$$a/c = n' \qquad (14)$$

$$S_{ya} = S_{yc}/\sqrt{n'} \qquad (15)$$

We then have:

$$n' = \left(S_{yc}/S_{ya}\right)^2$$

$$c = a/n' = a/\left(S_{yc}/S_{ya}\right)^2$$

By using equation (13), we find :

$$c = a/\left[S_{yC}/\left(\sqrt{a}S_{ya}\right)\right]^2 = \left[a\,S_{ya}/S_{yC}\right]^2 \qquad (16)$$

Proposition 6: S_{yC} is defined as the effective stress that acts on the macroscopic EAS. It must then correspond to the experimental stress S_y, which acts on the material. One has therefore:

$$S_{yC} = S_y \qquad (17)$$

By replacing in (16) and using (10), one finds:

$$c = \left[a\,S_{ya}/S_y\right]^2 = \left[aE/(2\pi S_y)\right]^2 \qquad (18)$$

- Calculation of macroscopic effective yield S_{yC}

We have:

$$S_{yC} = S_{yc}\sqrt{a} \quad \text{and} \quad S_{yc} = S_{ya}\sqrt{n'}$$

This gives:

$$S_{yC} = S_{ya}\sqrt{a}\sqrt{n'} \qquad (19)$$

Proposition 7: The dimension of c is an unknown fractal dimension:

$$c = a^k \qquad (20)$$

k is called the measure of recovery. One determines k as follows: $k = \log(c)/\log(a)$. c is given by relation (18). If proposition (7) is true, one should find k as constant. We also have from equation (14):

$$n' = a/c = a/a^k = a^{1-k} \qquad (21)$$

By replacing in equation (19), one finds finally the value of elastic limit of the macroscopic EAS:

$$S_{yC} = S_{ya}\,a^D = (E/2\pi)\,a^D$$
$$D = (2-k)/2 \qquad (22)$$

The results of experimental and theoretical values of elastic limits are shown in table 2. The experimental values are the cross reference values obtained from AISI, ASTM, FED, MIL SPEC, and SAE specifications but mainly from the excellent state of the art data given by Chaudron from his monographs on pure materials [16]. The experimental values given by the different sources sometimes vary significantly with very slight difference in purity, condition of production and testing. The values of k are also shown in table 2. Proposition 7 is verified since we find:

- For CC materials: $k = 1.618$ (23)
- for CFC and HC materials : $k = 1.47$ (24)

Mat.	a 10^{-10}m	E GPa	S_y MPa	S_{yC} MPa	c/a 10^{-5}	S_{yC}/S_y	k
Centred cubic Materials CC							
W	3.165	406	1000	977	0.13	0.97	1.62
Mo	3.147	310	720	745	0.14	1.03	1.61
Ti β	3.306	110	250	267	0.16	1.060	1.61
Pu	3.879	92	260	230	0.12	0.88	1.62
Centred faces cubic materials CFC							
Al	4.041	70	40	36	3.14	0.9	1.47
Ni	3.524	210	70	104	8.03	1.48	1.43
Cu	3.615	112	60	56	3.19	0.93	1.47
Ag	4.520	76	55	40	2.18	0.73	1.49
Pb	4.920	17	14	9,2	1.8	0.66	1.51
Hexagonal cubic materials HC							
Be	2.28 3.57	294	90	130	6.16	1.4	1.43
Mg	3.209 5.210	44	25	24	9.9	0.96	1.48
Zn	2.664 4.945	100	100	55	1.25	0.55	1.53
Sn β	5.831 6.491	41	15	22	11	1.46	1.43

Table 2: Values of experimental yield stress (S_y) and theoretical yield stress (S_{yC}).

The Scale Law of measure "SLM"

Equation (22) can be put in the following general form:

$$\boldsymbol{M}(L) = a^D\,\boldsymbol{M}(aL) \qquad (25)$$

with $\boldsymbol{M}(L)$ corresponding to S_{yC} and $\boldsymbol{M}(aL)$ corresponding to S_{ya}. This relation is called the SLM (Scale Law of Measure) relation. The SLM is a renormalisation process which gives a measure in scale by a measure in another scale. The generalisation to other measure has to be investigated.

Possible extensions of the theory

- Calculation of strain limit

The macroscopic strain limit can also be obtained as follows:

$$\varepsilon_{yC} = S_{yC}/E \qquad (26a)$$

By replacing S_{yC} by its value given by equation (22), we find:

$$\varepsilon_{yC} = (1/2\pi)\,a^D$$
$$D = (2-k)/2 \qquad (26b)$$

Table 3 shows the values of ε_{yC} for some materials. We get here nearly the limits of 0.2% of permanent strain which is admitted for the definition of the elastic limit for materials whose elastic limit is not well distinguished. We observe that physical strain limit has a pure geometrical value.

Mat.	a 10^{-10} m	ε_y
Al	4.041	0.0036
Ni	3.524	0.0020
Cu	3.615	0.0033
Ag	4.520	0.0046
Pb	4.920	0.0047

Table 3: Values of ε_y.

- Calculation of Toughness

The maximum stress on a point distant by r_f from the crack-front is given by the following relation:

$$\sigma_{11} = \frac{K_1}{\sqrt{2\pi r_f}} + ... \qquad (27a)$$

when r_f tends toward to the atomic dimension; in the limit case, we then have:

$$K_{ic} = S_{ya}\sqrt{\pi a} \qquad (27c)$$

We use a factor α to take into account the "defects" in the material and its ductility:

$$K_{ic} = S_{ya}\alpha\sqrt{\pi a} \qquad (27d)$$

The local toughness is equal to the global toughness from proposition 2. Equation 10 gives:

$$K_{ic} = \left(E / (2\pi)\right)\alpha\sqrt{\pi a} = \alpha E\sqrt{a / 4\pi} \qquad (27e)$$

The experimental values suggest an average value of 5 for α:

$$K_{ic} \approx E\sqrt{2a} \qquad (27f)$$

Table 4 shows experimental and theoretical K_{ic} values.

Mat.	a 10^{-10} m	E GPa	Kic Exper. MNm$^{-3/2}$	α	Kic theory MNm$^{-3/2}$	Theory/ Experience %
Tiβ	3.306	110	2.2	3.9	2.8	1.273
W	3.165	400	10	4.89	10.06	1.006
Al	4.041	70	2.0	5.0	1.99	0.995
Ni	3.524	214	5.9	5.2	5.7	0.996
Cu	3.615	112	2.7	4.49	3.0	1.111

Table 4: Experimental and theoretical values of fracture toughness.

- Calculation of fracture limit for ductile materials

To take into account the ductility of materials, a first approximation consists in introducing the phenomenon of plasticity at the atomic level and to take an atomic distance a^p instead of a. p is a coefficient of plasticity which lies between zero and one.

Equation (1) of Orowan: $S_{fa}^2 = E\gamma / a^p$ and equation [15] $\gamma = E a^p / (2\pi)^2$ give:

$$S_{fa} = E / (2\pi) \qquad (28a)$$

$$S_{fC} = E / (2\pi) \ a^{pD} \qquad (28b)$$

Some values of p are given in table 5. One notes that at the atomic level elastic fracture is the dominant mode of failure. For an exact analysis, it is necessary to use the following relation:

$$S_{fa}^2 = E\left(\gamma + \gamma_p\right) / a, \quad \text{with } \gamma_p >> \gamma \qquad (29)$$

Material	S_f	p
Al	200	0.70
Cu	400	0.66
Ni	400	0.71
Ag	300	0.68

Table 5: Values of p.

THE EXTENSION OF THE SLM TO NON PURE MATERIALS BY THE CONCEPT OF EFFICIENT ATOMIC DISTANCE

For non-pure material, the SLM can be extended to take into account the microstructure and the temperature effects by changing the value of the atomic distance a by the efficient atomic distance a_{eff} through the following relation:

$$\boldsymbol{M}(L) = a_{eff}{}^D \boldsymbol{M}(aL) \qquad (30)$$

We then have to study the change of the atomic lattice distance a_{eff} with microstructure and temperature. This study is beyond the scope of this paper. There is an abundant literature that gives a direct relationship between atomic lattice and microstructure effects for the numerous materials and solid solutions. Only some important illustrative results will be given below.

Effect of grain dimension

The factor of multiplication a^D is a universal factor. It can be used at any scale. We can then use it at the grain scale. Let's take the scale factor n instead of $1/a$ (which are equal from equation 11) and used it in equation 22:

$$S_{yC} = S_{ya} \ n^{-D} = \left(E / 2\pi\right)n^{-D}$$
$$D = \left(2 - k\right) / 2 \qquad (31)$$

The usual theories ignore the fractal dimension and then take (k=1 and then D=1/2). If we take an area of grain d and fill it with atom a, we then have: $na = d$ and therefore $n = d/a$. This gives a new SLM definition from the gain dimension as:

$$S_{yC} = S_{ya} \ a^D \ d^{-D} = \left(E / 2\pi\right)a^{1/2} \ d^{-1/2} \qquad (32)$$

We find the exponent of the grain size is $d^{-1/2}$; this correspond to classical theories like:

- The theory of Hall [6] and Petch [7]:

$$\sigma_f = \sigma_0 + Kd^{-1/2} \qquad (33a)$$

- The theory of Stroh [8]:

$$\tau_{eff} = \tau_y - \tau_i \geq \left[\frac{\pi\upsilon\gamma}{2(1-\nu)}\right]^{1/2} d^{-1/2} \qquad (33b)$$

- The theory of Cottrell [9]:

$$\sigma_f \geq \frac{2\upsilon\gamma}{K} d^{-1/2} \qquad (33c)$$

- Smith's relation [10]:

$$\sigma_f \geq \left[\frac{4E\gamma}{\pi(1-\nu^2)}\right]^{1/2} d^{-1/2} \qquad (33d)$$

We can identify equation (31) with the last theories (33 a-d) to get the values of the constants. In the case of Smith relation, if we use [15]: $\gamma = Ea/(2\pi)^2$ and by taking for example an average value of 0.3 for Poisson ratio, we find:

$$\sigma_f = 0,5\left(E / 2\pi\right)a^{1/2} d^{-1/2}.$$

This corresponds remarkably to our equation (31) by a factor of only 0.5.

Effect of atomic solid solution

In an atomic solution we have two materials A and B. The resulting average lattice distance depends on whether they are of the like kind, either both solvent or both solute or of the opposite kind. A first rule for the factor affecting solubility is given by Hume-Rothery [17]. This rule states that if the difference between atomic sizes exceeds 15%, solid solubility should become restricted. A size factor using the closest distance of approach can be used for the effective atomic size. Raynor [18] suggest a value of 100 $[(a_B-a_A)/a_A]$. The closest distance of approach sometimes does not express the lattice spacing in the solution (as in the case of Gallium for example). In this case, Axon and Hume-Rothery [19] have suggested an estimation of an apparent atomic diameter (AAD) and Massalsky and King [20] have suggested the measure of a mean atomic volume (Ω). They give the strain energy as:

$$W = A \, \mu \, \Omega \left(\frac{1}{\Omega} \frac{\partial \Omega}{\partial c} \right)^2 f(c) \qquad (34)$$

with A = constant, μ= bulk modulus and $f(c)$= function of composition c. For most alloys they find linear dependency of atomic volume with composition.

A model used for the calculation of the strain in solution is given by Eshelby [21]. In this model, the increase of volume (V_2) due to an increase of an internal cavity (V_1) is equal to:

$$\Delta V_2/\Delta V_1 = 3(1-v)(1+v) \approx 1.6 \qquad (35)$$

By using Vergard's law [22], which states a linear dependency on composition of lattice spacing, Friedel [23] has given an average atomic distance a for an infinite dilution and r for an finite concentration from initial atomic distance r_1 and r_2 of both the solvent and the solute:

$$\alpha = \frac{a-r_1}{r_2-a} = \frac{(1+v) \, X_1}{2(1-2v)X_2}$$
$$\frac{r-r_1}{C \, r_1} = \frac{r_2-r_1}{r_1} \frac{\alpha + (X_1/X_2)}{\alpha + 1} \qquad (36)$$

with X = compressibility and C = concentration.

The phenomenon of order-disorder (O-D) which influences the structure of solid solutions is also investigated throughout in the literature. Long-range order has been studied and reviewed by Guttman [24]. The condition of order is that dissimilar atoms must attract each other more than similar atoms in order to lower the free energy. This conditions is expressed as:

$$E_{AB} < 1/2 \, (E_{AA}+E_{AB}) \qquad (37)$$

If r is the fraction of A atoms in the alloy and p is its probability to occupy a site, long range order S is then defined by Bragg and Williams as [25]:

$$S = (p-r) / (1-r) \qquad (38a)$$

If q denotes, the fraction of unlike nearest neighbours and q_r and q_m are the fractions of unlike nearest neighbours at conditions of maximum randomness and maximum order, then short range order is defined by Beth as [26]:

$$S = (q-q_r) / (q_m-q_r) \qquad (38b)$$

Lattice distances in solid solution are already available from the voluminous data given by Pearson [27]. Pearson shows that changes in lattice spacing influences also the magnetic properties.

Other effects (temperature, impurities, etc.)

Numerous relations show the correlation between crystalline dimensions and these effects. We can only mention some of them. The effect of temperature for Copper is given by Mitra [28]:

$$a_t = 3.6193 + 5.81 \; 10^{-5} \; T + 3.7 10^{-8} \; T^2 - 5.2 \; 10^{-11} \; T^3 \quad (39)$$

For phase α of Ti, Schmitz [29] provide tables, which give the variation of a_t with temperature. For phase β, Medoff [30] gives the following results:

$$a_t = a_0 [1 + 9.928 \, (t\text{-}25) \; 10^{-6} - 0.626 \, (t\text{-}25^2) \; 10^{-10}] \quad (40a)$$
$$c_t = c_0 [1 + 11.079 \, (t\text{-}25) \; 10^{-6} - 9.698 \, (t\text{-}25^2) \; 10^{-10}] \quad (40b)$$

The effect of impurity for phase β of Titanium is given by Wassilewsky [31] who shows that lattice parameters (c/a) increases from 1.59 to a limit of 1.63 for an equivalent increase of O_2 concentration from 0 to 0.5%.

DISCUSSIONS

Results of yield stress

- Table 2 shows that the mean value of S_{yC}/S_y is found to be equal to 0.99. This result is exceptional since the classic theories [1,2,3,4] based on the model of Orowan give error of the order of 10^2 to 10^4.

- Relation (22) of theoretical elastic limit confirms proposition n°3 of "geometrisation" of physics. The scale factor n is actually related to the material by the relation: $n=1/a$. The factor a represents really the atomic "dimension" and not only the atomic distance since it takes into account the density of the material by an optimal stacking.

- the value of k given is for large scale (passage from the microscopic to the macroscopic world). For two values belonging to the same world, say macroscopic world, we then have:

$$(S_{yC})_1 = S_{ya} \, n_1^{-D} \text{ and } (S_{yC})_2 = S_{ya} \, n_2^{-D}$$

then:
$$(S_{yC})_2 = (S_{yC})_1 \, n^{-D}$$

If: $k = 1$, then $-D = -\frac{1}{2}$. We find then relation (9).

- We can notice that ratio c/a (which measures the degree of compactness or fill) is lower for CC materials whose compactness is 68%. This degree is higher for CFC and HC materials whose compactness are 74%. The ratio $(c/a)^2$ or a^{2k}/a^2 is the degree of fill. If $k = 1$ then $a = c$. It is this confusion that make the classical analyses confound matter with the atom whereas matter is rather in the microscopic EAS. The factor of multiplication a^D is estimated between 10^{-2} and 10^{-4} corresponds precisely to the degree of error of the classic analysis. The ratio c/a is the order of 10^{-4} to 10^{-6}. This value corresponds to the ratio of the core to the atom, which is actually in the order of 10^{-4}. The EAS could then represent the dimension of the atomic core or the dimension

of any elementary particle. The exact calculation between c and the core could indicate the existence of void in the core, which is physically admissible.

- Petch relation supposes that we can extrapolate the grain size to the atomic dimensions and hence obtain the yield at the atomic scale. Christ [32] has shown that this is not true. This can be explained by the fact that the fractal dimension changes with scale. At the grain size, $k = 1$ and $D = 0.5$ wile at the nanoscale and atomic scale $k = 1.6$ and $D = 0.2$.

Insurance Quality (IQ) tests and simulation tests

Even though tests always remain standards, the value of k (and therefore S_y) depends on the microstructural state of the material, temperature, method of production and the damage, which occurred during its length of life. The difference between experimental and optimum values given by equation (23) can constitute an IQ criteria to appreciate the quality of the material. As the methods of productions are improved, k values will tend toward the given theoretical values. These optimal values can never be (theoretically) exceeded. With the theoretical determination of S_y, it becomes unnecessary to make destructive testing for the characterisation of the material. An NDT which give the lattice dimension will be sufficient when used with the SLM. It will also not be necessary to make expensive simulation tests to get the change of propriety by scale.

Universal Measure through scale factor

The procedure pursued to determine the macroscopic Measure S_y is a standard procedure that can be (theoretically) applied to any physical Measures (temperature, pressures, energy, etc.) where exist a difficulty to get a macroscopic measure from its microscopic measure and inversely!. These concern critical passages as bifurcation, transition between critical flow in fluid mechanics and aerodynamic, whirls, bursting of whirls, instabilities, privileged angles in aerodynamics or in botanicals, chaos and disorders, etc. The SLM depend only on the scale factor a^D or n^{-D} which can be used as a factor of normalisation to gives the variation of any measure with scale.

CONCLUSION

The presented SLM theory strikes by its simplicity, its precision and its concepts (gometrisation and scale factor) that can be generalised to other measures. The SLM has been used for the theoretical determination of the elastic limit of pure materials. The mean of experimental over theoretical (S_{yC}/S_y) value is found to be 0.99. This result is exceptional since the classic theories [1,2,3,4,5] based on the model of Orowan give an error of the order of 10^2 to 10^4. The best theories are the one that stops at the grain level (Petch, Hall, Stroh, Cottrell, Smith) and which can be viewed as special cases of the SLM.

It is found in this study that the microscopic EAS is also a good representation of the atomic core where it gives a new representation of the microscopic world as a fractal

world. The main result of this paper shows that the atomic distance is the key factor for characterisation of the materials. At this level (the Amstrong scale), very small distance differences can make significant differences in the characteristics (mechanics but surely also magnetic, optical, chemical or electronic characteristics) of the materials. This is of a fundamental result in physics.

The possible extension of the SLM to give new relations for the elastic limit of strain, the toughness and the fracture strength has been investigated. The results seem acceptable, but future work has to be done to fully investigate these relations.

A suggestion for the extension of the SLM to take into account the microstructure (grain size, impurity, phases, solutions, etc.) and the temperature effects is given through the concept of an "efficient atomic distance" which represents the affected new lattice spacing.

The generalisation of the SLM relation to other physical measure is to be investigated to see if this relation can be used as a universal criterion which gives the scale or the size effect on physical measures for "renormalisation" schemes. This could lead to new design for high performance materials by conceiving materials with high "efficient atomic dimension".

NOMENCLATURE

A^2	Apparent macroscopic area under stressing.
a^2	Apparent microscopic area under stressing.
a	Atomic crystal lattice dimension.
a_{eff}	Efficient atomic distance (dimension).
b_1, b_2	Constants of repulsion.
B_1, B_2	Constants of energy.
C^2	Effective macroscopic area under stressing.
c^2	Effective microscopic area under stressing.
D	Fractal parameter.
d	Grain size.
E	Young (elastic) Modulus.
F	Force.
K	Stiffness.
K_1	Stress intensity factor (mode I).
K_{ic}	Toughness (mode I).
k	Measure of recovery for the fractal dimension of "c".
M	Constant of Madelung.
$\mathbf{M}(L)$	Measure of a quantity "L".
n	Scale factor between A and a (= A/a).
p	Coefficient of plasticity.
n'	Scale factor between a and c (a/c).
r	Distance between atoms.
r_f	Distance front crack front.
r_0	Equilibrium distance between atoms.
S_y	Experimental yield (or elastic) stress.
S_{ya}	Microscopic apparent yield stress acting on apparent microscopic area "a^2".
S_{yc}	Microscopic effective yield stress acting on effective microscopic area "c^2".
S_{yA}	Macroscopic apparent yield stress acting on apparent macroscopic area "A^2".
S_{yC}	Macroscopic effective yield stress acting on effective macroscopic area "C^2".
S_f	Experimental fracture limit (or ultimate strength).
S_{fa}^2	Fracture limit (or ultimate strength) on apparent microscopic area "a^2".

S_{fC}^2 Fracture limit (or ultimate strength) on effective macroscopic area "C^2".

U_a Coulomb energy of attraction at atomic level.

U_r Potential energy of repulsion at atomic level.

U Total energy at atomic level.

z Number of neighboring atoms.

α Factor of defect for toughness calculation.

σ_f Failure stress.

τ_f Shear failure stress.

γ Free surface energy for elastic mode of failure.

γ_p Free surface energy for plastic mode of failure.

ϖ Factor of Coulomb $\varpi = q^2 / (4\pi\varepsilon_0)$.

ε_0 Dielectric constant in vacuum.

ε_{yC} Macroscopic strain limit.

ξ Orowan factor.

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