A MICROSTRUCTURAL APPROACH TO THE TENSILE STRENGTH OF CARBON MATERIALS WITH DIFFERENT TEXTURES

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Introduction

In 1997 one of the authors (FGE) presented a paper at the Carbon 1997 conference [1], to study the fracture of polygranular graphites. In the end of that paper it was observed that the mean calculated surface energy by using the Griffith theory [2] should be regarded as an effective (or apparent) surface energy and that an analysis based on an atomistic approach (Ref #8 of [1]) could clarify some discussed aspects and be useful in the study of the fracture of other materials.

Although the basic aspects of Ref. # 8 of [1] were known, careful experiments [3] had to be performed to arrive at "a new approach to the fracture of brittle solids considering the microstructure and atomicity", which is being submitted to publication [4].

In this work we are applying the new developed approach to analyze in a new perspective the fracture of the carbon materials which were the starting point of our concerns. These materials (H-451, IG-110, AXF-5Q), studied previously by Burchell [5], are respectively medium, fine, and ultrafine polygranular graphites with bulk density of about 1.78 gcm^{-3} and Young's modulus of about 10.6 GPa.

Application of the developed theory

In Ref. [4], it is shown that the beginning of a fracture can be determined by the reaching of a specific maximum value of the local stress between the unit cells (or grains, in cases of polygranular materials) at the extremity of a critical flaw. It is obtained an expression for the tensile strength (σ_{TS}), defining an effective microscopic cleavage stress ($\sigma_{eff.}$). The general expression for (σ_{TS}) depends on $\sigma_{eff.}$ and the stress concentration factor K_m due to almost the whole flaw, which may present dimensions from a macroscopic scale (for large flaw sizes) down to a usually microscopic radius of curvature ρ_m. The other stress concentration factor (K_a) is due to the part of the flaw close to the exact local where the rupture begins, which presents dimension of the order of a few multiples of λ (the characteristic dimension of fracture). In the case of the carbon materials λ is of the order of the interlayer spacing of graphite (0.335 nm).

For cases of plane stress (for example, by using a thin plate) with a transverse flaw where additionally it may be possible to apply the concept of equivalent ellipse [6,7], the theoretical expression for the tensile strength may be approximated by:

$$\sigma_{TS} = (\sigma_{eff.}/2)\ (\rho_m/a)^{1/2} \qquad (1)$$

Although the studied material cannot be regarded as strictly submitted to a case of plane stress, presenting 3D pore flaws, we will apply equation (1) as an approximation, which has to be duly corrected to take into account the 3D nature of the material and their flaws.

The flaw distribution, orientation, and length related to the fracture can be treated as in Ref. [1]. According to equation (1), if a body contains flaws of different lengths, then the larger flaws are expected to control the strength. Since the scattering of brittle strength measurements indicates that the number of dangerous flaws cannot be very large [8], the critical flaw size ($2a$) will be taken equal to the length of the fail situated at 99.9% of the log-normal distribution of the flaw size statistic [5], that is, only 0.1% of the fails may have length above $2a$. In Table 1 we give the experimental values of σ_{TS} and of $2a$ of the materials.

Results and Discussion

Since the experimental relationship of σ_{TS} as a function of $(1/a)^{1/2}$ is well represented by a straight line that passes trough the origin (cf. Fig. 1), then, according to equation (1), the angular coefficient $(\sigma_{eff.}/2)\ (\rho_m)^{1/2} = 2.03 \times 10^5\ Nm^{-1/2}$ is a constant for the studied materials.

If we assume that the materials present similar configurations at the atomic scale where the rupture starts, then a good assumption is to consider $\sigma_{eff.}$ constant. The value of $\sigma_{eff.}$ can be estimated from the value of the critical local maximum stress ($\sigma_{local\ max.}$) where the rupture does begin to occur - which corresponds to the so called theoretical strength (which is of the order of (E_c/π) [9]) - and the values of K_a and c_{ma} (the coupling constant between K_m and K_a [4]). Since E_c = 36 GPa, we can show that $\sigma_{eff.}$ ~ 10 GPa for the case of the polygranular graphites. Consequently, ρ_m ~ 1.6 nm; this value corresponds approximately to 5 c_o (five atomic interlayer spacing of graphite), which is coherent with the atomistic characteristic of the fracture process. As emphasized in Ref. [4], we would commit a mistake if we take the radius of curvature decrease to zero indefinitely, as performed in other approaches.

Another point that can be mentioned is that the surface energy calculated by using a simplified expression of Kelly-Macmillan (eq. 1.10 of [9]) and those of the developed approach [4], give values of 3.9 and 3.6 $J.m^{-2}$ respectively, which are below the values reported previously for the effective (or apparent) surface energy ($\gamma_{app.}$= 6.6 Jm^{-2} [1]).

Finally, it is important to observe that Mrozowski Cracks (formed by anisotropic contraction on cooling from graphitization temperatures) located at the extremity of the critical flaws play an important role in the delimitation of the region of K_a and in the fracture properties of the studied materials.

Table 1. Tensile strength [5] and critical flaw-size [1] of polygranular graphites.

Material	σ_{TS} (MPa)	$2a$ (m)
H-451	16.0 ± 1.6	3.7×10^{-4}
IG-110	25.7 ± 1.9	1.4×10^{-4}
AXF-5Q	65.1 ± 5.5	1.9×10^{-5}

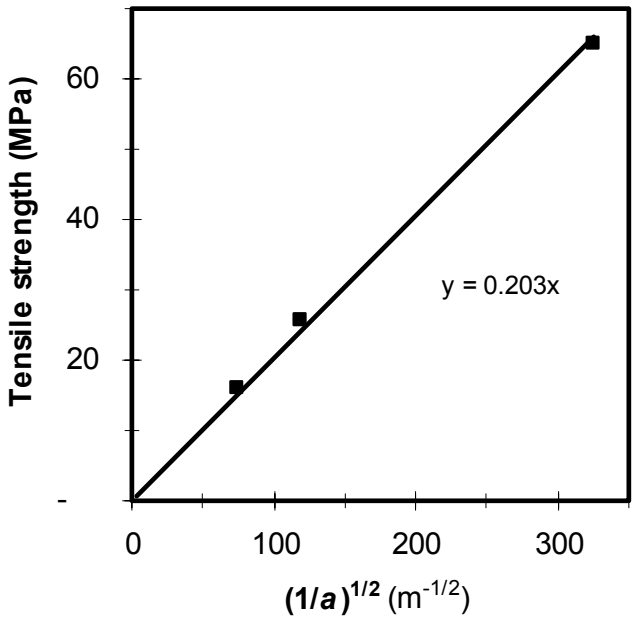

Fig. 1 – Tensile strength as (σ_{TS}) of polygranular graphites as a function of $(1/a)^{1/2}$.

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