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On the use of partial properties to interpret the bulk crack propagation behaviour of coarse two-phase materials

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The principle of partial properties is applied for the derivation of bulk properties of materials which contain more than one structural element. Partial properties are the particular properties of these elements from which together with volume portion, morphological dimension and geometry properties concerned with critical and subcritical crack growth are derived for certain micro-structures in metals as well as polymers.

1. Introduction

Coarse two-phase structures are distinguished here from fine two-phase structures, which are for example, alloys in the state of precipitation hardening, as caused by particles in the order of magnitude of 1 to 10 nm. The dimensions of coarse structures are more than 10^2 times larger ($\gg 1$ μm). The term "phase" is not necessarily applied in a strict sense. An area with an unique mechanical behaviour (for example tempered martensite or an even mixture of crystal and glass) can be included into these considerations. The microstructural species can be classified as dispersion, net, duplex and dual-phase structures using grain and phase boundaries as topological features in addition to the volume portions (Table 1) [1].

Such structures can be recognized in metallic [2] as well as in polymeric materials [3]. There are some efforts to interpret yield stress and plastic deformation behaviour of coarse two-phase structures using equations in which volume portions f_i and properties of the phases $\bar{p}_i$ are contained to obtain predictions on the property P of the bulk alloy [4–6]. For complex microstructures, for example ferrite–pearlite, finite element calculations have been used to simulate the inhomogeneities of plastic deformation [7].

The term partial property is used for the properties of the individual microstructural elements which are composed of a coarse two-phase structure. There have already been some efforts to use this concept to explain the crack propagation behaviour of such structures, for example, for critical crack growth of precipitation hardened alloys with soft zones in the environment of grain boundaries [8, 9], coarse spherulitic structures of thermoplastic polymers [10, 11], and for the fatigue and critical crack growth in duplex- and dual-phase structures of nickel steels [12, 13]. It is the objective of this paper to define the conditions under which the concept of partial properties is useful to interpret bulk fracture mechanical properties.

2. Bulk deformation

The situation of constant strain across the cross section is used to find simple functions between bulk property, partial properties and volume portions

$$P = F(\bar{p}_i ; f_i) \qquad (1)$$

The rule of mixtures

$$P = \bar{p}_\alpha \cdot f_\alpha + \bar{p}_\beta \cdot f_\beta \qquad (2a)$$

is obtained for the elastic modulus and parallel lamellae of α and β (Fig. 1)

$$E = \bar{E}_\alpha \cdot f_\alpha + \bar{E}_\beta \cdot f_\beta \qquad (2b)$$

for all stresses $\sigma_\alpha \neq \sigma_\beta$ smaller than the yield stresses of the phases. In the case of a sequential arrangement of α and β the plastic deformation ϵ in direction of the stress σ is described by this equation if the yield stress of both phases is transpassed ($\sigma > \bar{\sigma}_{y\alpha}$; $\sigma > \bar{\sigma}_{y\beta}$)

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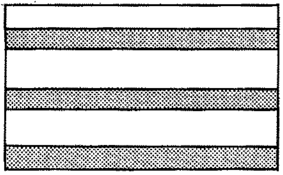
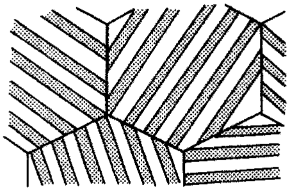
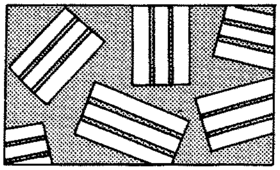
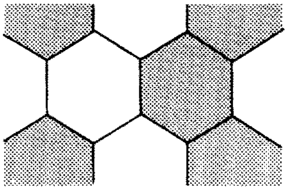
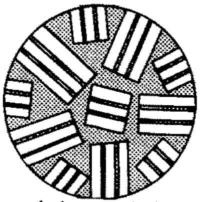
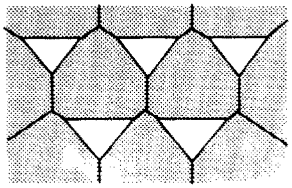
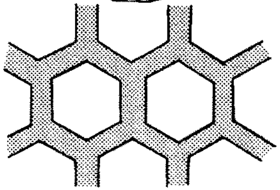
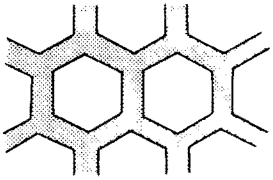
TABLE I List of morphological elements in polymers and structural elements in metals.

No.	Morphological element	Symbol	Structural element	Symbol
1	Folded Chain Crystal (β)	☐	Hard phase (β)	☐
2	Random coil structure (α)	▨	Soft phase (α)	▨
3	Package of folded chain crystals (β) with amorphous intercrystalline structure		Grains with lamellar microstructure of (α) and (β)	
4.	Randomly distributed packages (β) with random coil structure (α) between		Statistical distribution of grains (α) and (β) with the same size i.e. Duplex structure	
5.	Spherulite with radially arranged packages (β) and amorphous structure (α)		Distribution of phase (β) at triple-points of grains of phase (α) i.e. Dual phase structure	
6.	Polygonal structure of spherulites (β) with amorphous interspherulitic layer (α)		Matrix of phase (β) with phase (α) only at grain boundaries i.e. net structure	

$$\epsilon = \bar{\epsilon}_\alpha \cdot f_\alpha + \bar{\epsilon}_\beta \cdot f_\beta. \tag{2c}$$

If only one phase is plastically deformed, bulk deformation depends on the partial property on one phase only ($\bar{\sigma}_{y\beta} > \sigma > \bar{\sigma}_{y\alpha}$)

$$\epsilon = \bar{\epsilon}_\alpha \cdot f_\alpha \tag{3a}$$

in general terms

$$P = \bar{p}_\alpha \cdot f_\alpha. \tag{3b}$$

The fracture stress of the same arrangement of phases is even independent of the volume portion and equal to the fracture stress of the weaker phase ($\bar{\sigma}_{F\beta} > \bar{\sigma}_{F\alpha}$)

$$\sigma_F = \bar{\sigma}_{F\alpha} \tag{4a}$$

in general terms

$$P = \bar{p}_\alpha. \tag{4b}$$

3. Crack Propagation

3.1. Extreme cases

The rule of mixtures (Equation 2a) should be suitable for a structure in which both structural elements contribute portions of the fracture surface which are equal to the ratio of the volume portions. This condition is fulfilled for a crack which propagates without deviations perpendicular to the direction of the external load (Fig. 2). The crack extension energy G_{IC} for a crack with a straight tip under these conditions is

$$G_{\text{IC}} = \bar{G}_{\text{IC}\alpha} \cdot f_\alpha + \bar{G}_{\text{IC}\beta} \cdot f_\beta. \tag{5}$$

The validity of this relationship has been confirmed in duplex structures of Fe–Ni–alloys[12, 13]. In the temperature range of the transition to brittleness there is however a tendency to a higher toughness of the α-phase in the duplex structure as

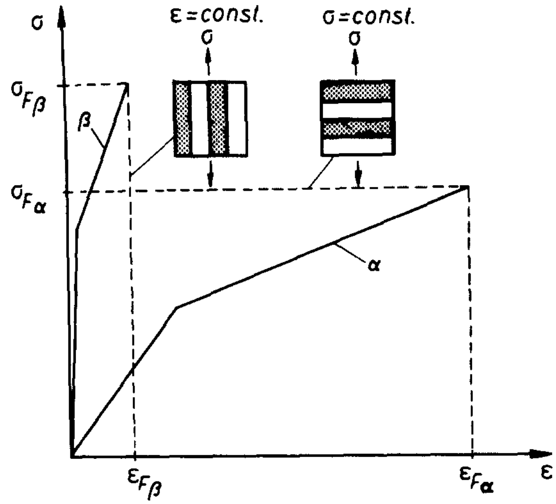


Figure 1 Schematic stress–strain curves of elements 1 and 2 (compare Table 1).

compared to the same phase in the bulk $\bar{G}_{IC\alpha} > G_{IC\alpha}$.

For structures of the net and the dispersion type (Table I) one phase can be completely or partially by-passed by cracks. An almost complete avoidance of the microstructural element β is observed for subcritical crack growth of coarse-spherulitic PP (Polypropylene)[10, 14] and for fatigue crack growth of low temperature Fe–Ni–steels [12] (Fig. 3).

If the crack propagates exclusively in the soft α-phase (a low molecular weight, amorphous interspherulitic material) the bulk properties are determined only by $\bar{G}_{IC\alpha}$. As the plastic zone size r_p [15] is much larger than the thickness of this layer ($D \sim 1 \mu m$), only its small volume portion f_α contributes to energy dissipation and therefore to toughness (Fig. 4). It is, however, modified by the molecular weight (MW) of the polymer. An increase of MW leads to more interspherulitic links [16], which provide a higher degree of plastic deformation before fracture in the interspherulitic zones (Fig. 5). The result is an increase in the partial property $\bar{G}_{IC\alpha}$.

Finally it is necessary for the crack to be diverted from the normal direction by an angle ϕ, so that a smaller component of the external stress $\sigma_{eff} = \sigma \cdot \cos\phi$ becomes effective. This requires a geometric factor $g > 1$ which is determined by the details of the morphology and an average of all ϕ_i. Thus g accounts the extra path around the phase β.

$$G_{IC} = \bar{G}_{IC\alpha} \cdot f_\alpha \cdot g. \qquad (6)$$

The situation is different, if the plastic zone is smaller than the dimension of a microstructural element: $r_p < D$. This is verified for example by low amplitude fatigue crack growth (Fig. 6). Then the bulk property becomes independent of the volume portion f_α. Only the geometrical factor g is still required to take care of the local deviations of the crack

$$\frac{da}{dn} = \left(\frac{\overline{da}}{dn}\right)_\alpha \cdot g^{-1} \qquad (7)$$

da/dn is the crack growth per cycle for a certain dynamical loading condition. Equations 6 and 7 correspond to 3 and 4. It may be emphasized that the

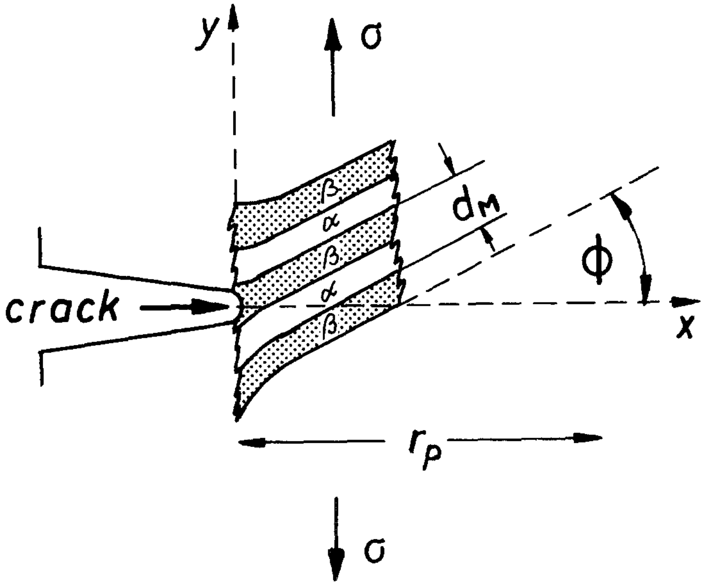


Figure 2 Element 3 (compare Table 1) at the tip of a crack.

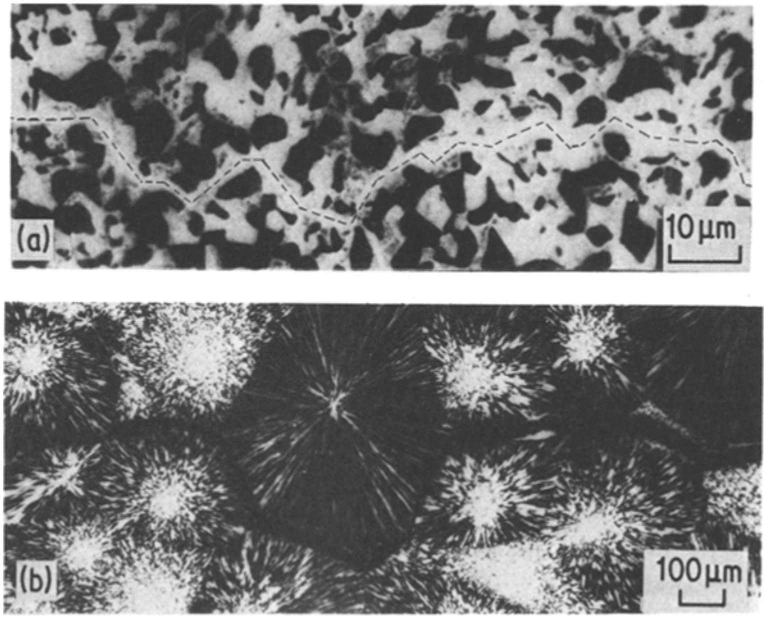


Figure 3 (a) Fatigue crack path (dotted line) along the white etched, soft phase (α) in a duplex-structure of a Fe–Ni–alloy (Fe–9% Ni). (b) Crack propagation along spherulite boundaries in coarse-spherulitic Polypropylene.

ratio of the dimension of the reaction zone r_p to microstructural dimensions D is an additional important factor which determines the applicability of the Equations 2a, 3b and 4b.

3.2. Intermediate cases

The prerequisites for the validity for the Equations 5 to 7 are often not fulfilled, because a crack may pass through α only up to a critical angle ϕ_c. At higher angles the orientation of α becomes unfavourable, so that β can be passed. In this case neither Equation 5, 6 nor 7 are valid. This intermediate condition can be quantitatively expressed by the critical angle ϕ_c above which a crack starts to pass in the second phase β. This angle can be easily determined experimentally as it is shown schematically for the case of a net structure (Fig 7).

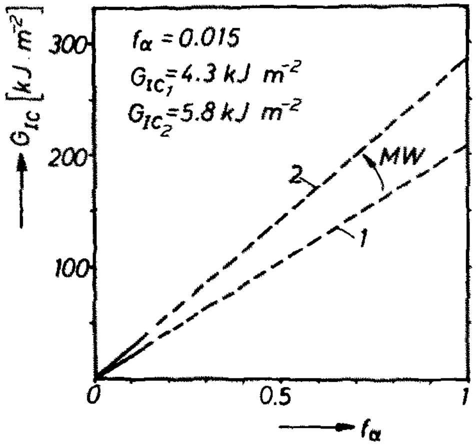


Figure 4 Crack extension force of mixtures of two kinds of PP with different molecular weights MW and coarse-spherulitic morphology.

Fig. 8 also gives the example for the transition from inter- to trans-spherulitic crack propagation in PP and for the corresponding case of mixed inter- to trans-granular fracture in a precipitation hardening aluminium alloy with narrow particle free zones as grain boundaries.

Assuming that a crack tends to move preferredly in α, the effective amount of β which is passed, is reduced for $\phi_c > 0$ by a factor $0 \leqslant a \leqslant 1$

$$\left(1 - \frac{2\phi_c}{\pi}\right)\cdot f_\beta = f_\beta^* = a\cdot f_\beta \tag{8}$$

Only for $\phi_c = \pi/2$ the crack passes exclusively α and Equations 6 or 7 become valid.

Under the conditions for the validity of Equations 4b and 7 i.e. for a small plastic zone $r_p < D_\alpha$, the effective volume portion of α passed by the crack is

$$f_\alpha^* = 1 - f_\beta^*. \tag{9}$$

Equations 2 and 5 must be supplemented

$$P = \bar{P}_\alpha\cdot f_\alpha^*\cdot g_\alpha + \bar{P}_\beta\cdot f_\beta^*\cdot g_\beta \tag{10}$$

to consider the real behaviour of the crack including the average angular deviations by geometrical factors g_i.

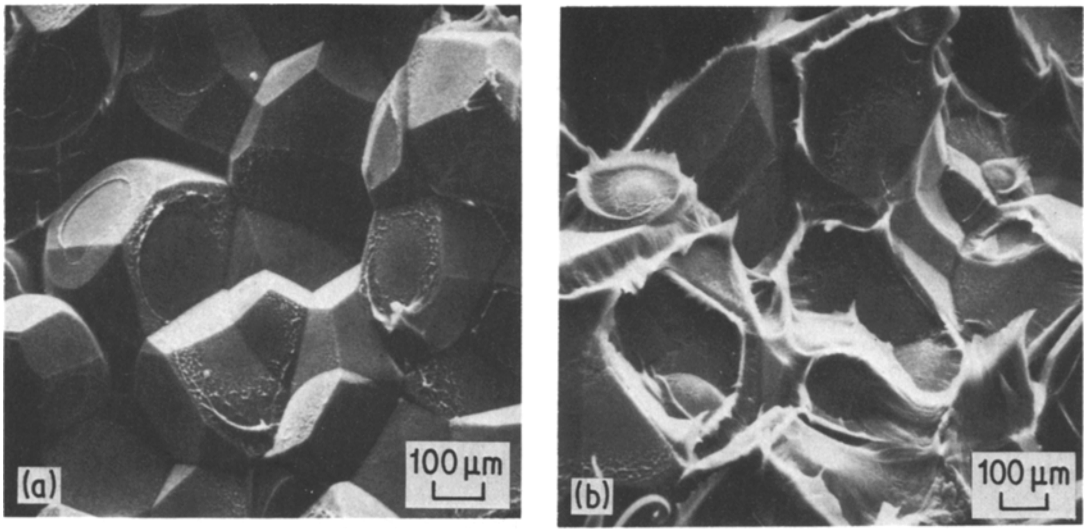


Figure 5 Interspherulitic fracture surfaces of coarse-spherulitic Polypropylene with (a) a lower and (b) a higher molecular weight. (compare lines 1 and 2 in Fig. 4).

An inspection of the basis for the applicability of Equation 10 shows, that for $r_p > D_\alpha$ Equation 9 is no longer valid

$$f^*_\alpha + f^*_\beta \neq 1 \qquad (11)$$

because f^*_α can vary between f_α and 1 (Equation 3 and 6 and 4 and 7). The transitional behaviour between $r_p < D_\alpha$, i.e. low amplitude fatigue, and $r_p > D_\alpha$, i.e. critical crack growth of a material with large plastic zone, can be described by introducing a factor b. This is controlled by the ratio of the dimension of the plastic zone required by fracture mechanics r_p, to that provided by the microstructure D_α (Fig. 9)

$$f_\alpha^{-1} \geqslant b \geqslant 1 \qquad (12)$$

A fatigue crack for example may pass through all these limits as it grows and increases its plastic zone. Consequently different growth mechanisms and growth laws apply. Using the factor b and including the geometrical factor, Equations 3 and 4 as well as 6 and 7 may be writted in general terms as

$$P = \bar{p}_\alpha \cdot f_\alpha \cdot b \cdot g_\alpha \qquad (13)$$

and for the most general case that in addition a portion of β is passed by the crack

$$P = \bar{p}_\alpha \cdot f_\alpha \cdot b \cdot g_\alpha + \bar{p}_\beta \cdot f_\beta \cdot a \cdot g_\beta \qquad (14)$$

with $\Sigma f_i = 1$.

Finally it has to be noted that ϕ_c and therefore a (Equation 8) is a function of the ratio of the partial properties $\bar{p}_i$. For deformation and separa-

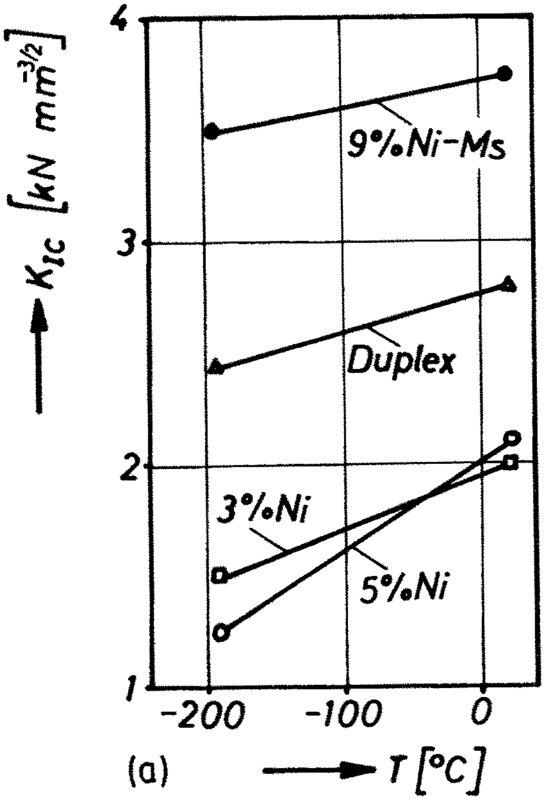
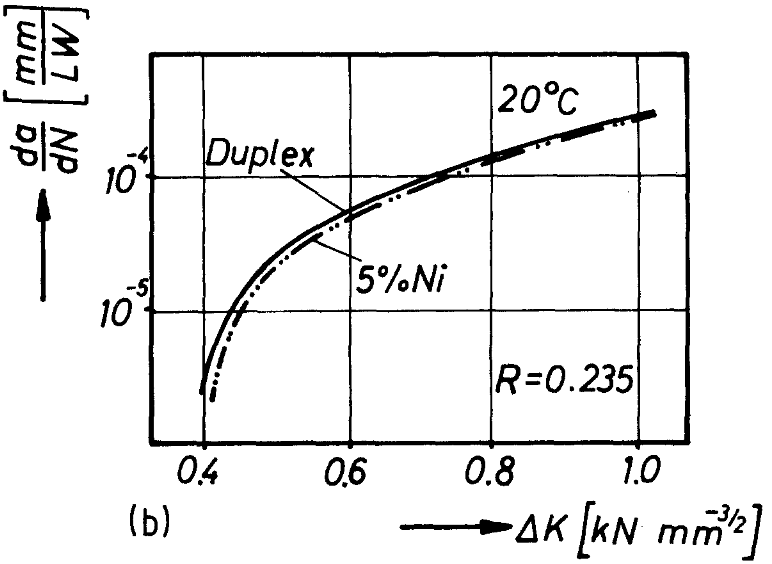


Figure 6 (a) Fracture toughness K_{IC} versus temperature of various structures in Fe–Ni–alloys. (b) Fatigue crack growth diagram of an Fe–5% Ni–alloy with either duplex structure or as homogeneous solid solution.

Figure 6 (*continued*)



tion directly induced by the normal stress the component of the external stress in α which is inclined to the direction of this stress by ϕ becomes equal to the normal stress necessary for crack propagation in α for

$$\frac{\bar{p}_\alpha}{\bar{p}_\beta} = \cos\phi_c. \qquad (15)$$

If the separation takes place by shear, orientations which provide maximum shear stress ($\phi = \pi/4$) and not $\phi = 0$ are the optimum and different critical angles are expected. This is for example found for precipitation hardened aluminium alloys, where plastic intercrystalline separation occurs by normal as well as shear stress. Measurements of ϕ_c can be used to determine partial properties or at least their ratio experimentally. This in turn provides a way to test data by physical models for these elementary structures of which the microstructure of the bulk material is composed. Finally it should be mentioned that these concepts together with suitable geometrical factors are also suitable to further treat microstructural details of crack propagation anisotropy in alloys or passage of a crack through a spherulite in polymers.

4. Conclusions

Partial properties are properties of structural elements such as phases, or ultra fine microstructures which can be regarded as behaving mechanically homogeneous such as precipitation hardened crystals, tempered martensite and (to a lesser degree) the interior of spherulites of which a microstructure is composed. It is discussed how bulk fracture mechanical properties P can be obtained from partial properties $\bar{p}_i$, volume portions f_i, and microstuctural dimensions D_i and geometry, The bulk behaviour may be determined as limiting equations by the rule of mixtures

$$P = \bar{p}_\alpha \cdot f_\alpha + \bar{p}_\beta \cdot f_\beta$$

or by one phase and its volume fraction

$$P = \bar{p}_\alpha \cdot f_\alpha$$

or by the bulk properties of one phase alone

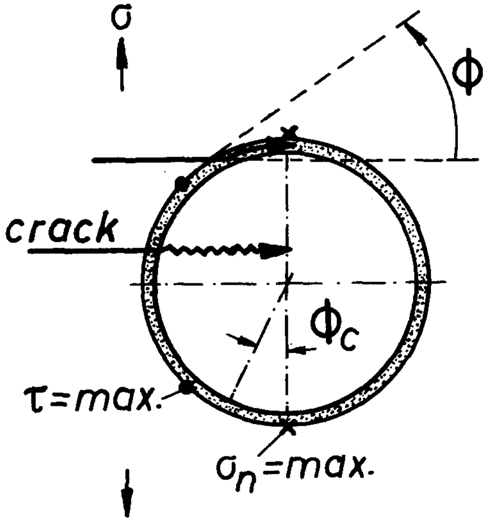


Figure 7 Possible orientations of the interspherulitic layer (α) to the external load. The angular range of inter- ($\phi < \phi_c$) and trans-spherulitic crack growth is indicated.

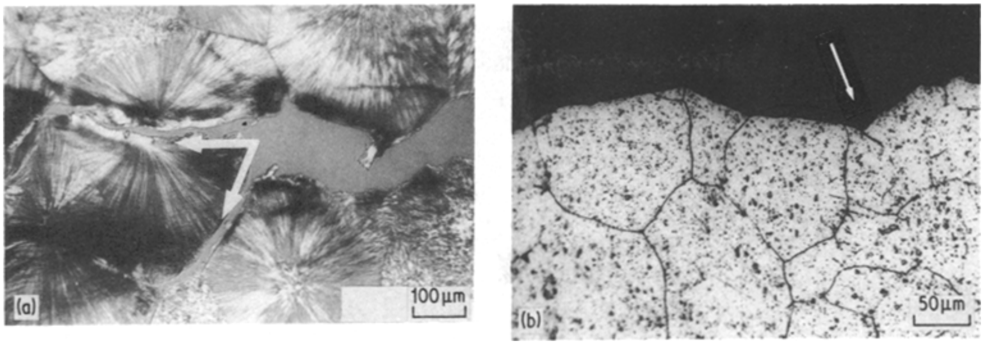


Figure 8 (a) Bifurcation of a crack into an inter- and trans-spherulitic path in a coarse-spherulitic structure of PP with

$$P = \bar{p}_\alpha$$

There exist transitional conditions between these extreme cases which are controlled by the ratio of the partial properties $\bar{p}_\alpha/\bar{p}_\beta$ for crack propagation and by the ratio of plastic zone size r_p and dimensions of microstructural features D_α, $r_p \lesseqgtr D_\alpha$. A factor $0 \leqslant a \leqslant 1$ is applied to consider a decreasing portion of crack propagation through β, while for $a = 0$, a factor b takes care of the fact that the macroscopic property P becomes dependant or independent of the volume portion of α, f_α. A microscopic method for the determination of partial properties is discussed by which physical models for the prediction of properties of the

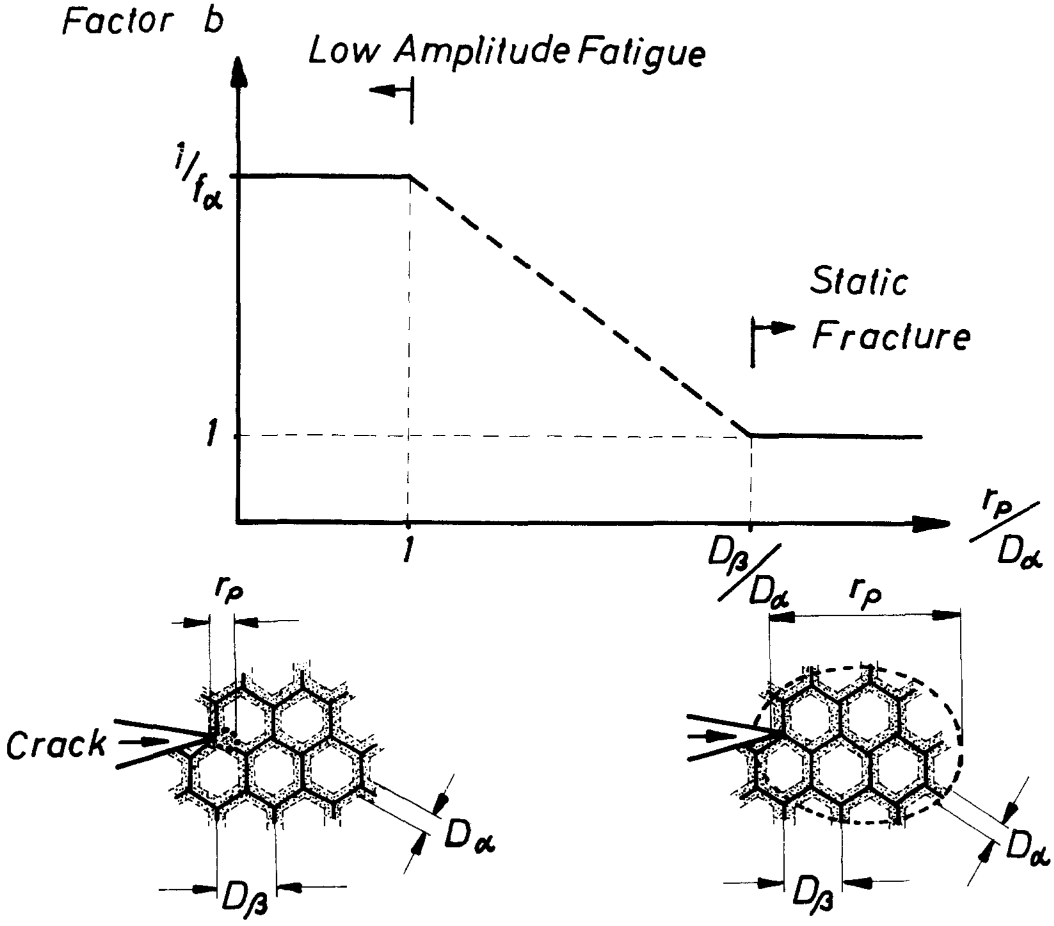


Figure 9 Correlation between fracture mode, plastic zone size r_p and factor b, by which the ratio of r_p/D_α is controlled.

structural elements may be tested. This can be useful if these structures cannot be produced in bulk as is case for semicrystalline polymers.

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