Mechanism of in-plane fracture growth in particulate materials based on relative particle rotations

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Abstract In-plane fracture propagation in particulate materials (rock, concrete) under high tri-axial compression is observed in both Mode I tensile cracks (opened by additional load), Mode II shear cracks and in Mode I anti-cracks (compaction bands). This commonality suggests that when the conventional fracture mechanisms are supressed by high compression, a new universal mechanism takes over. We propose a fracture growth mechanism based on mutual rotations of the particles leading to breakage of inter-particle bonds followed by particle detachment and re-compaction. The Cosserat characteristic lengths are found to be of the order of the particle size. This allows expressing the stress concentrations as an intermediate asymptotics (between the Cosserat continuum characteristic length and the crack length). For Mode I crack and anti-crack and for Mode II crack the stress singularities are the same as for the cracks in a classical continuum, while the moment stress has a stronger singularity (3/2 power). This stress singularity leads to relative particle rotations and bending of interparticle bonds. The tensile microstress induced by the bending is an order of magnitude higher than the stress associated with conventional stress singularities.

Keywords Fracture Criterion, Grain rotation, Moment stress, Small-scale Cosserat continuum, Compaction band

1. Introduction

Fracture mechanics recognises 3 main fracture modes, one tensile (Mode I) and two shear (Modes II and III). Numerous experiments show that in brittle and quasi-brittle materials without pronounced planes of weakness, Mode I cracks are capable of in-plane growth, that is growing in their own plane, while Mode II cracks kink. In rock fracturing in compression however two more phenomena are observed. Firstly, it is in-plane propagation of shear bands; they start at near the peak load and propagate at an angle to the load direction throughout the rock sample separating it into two parts. This zone looks like shear (Mode II) crack (e.g. [1-3]) and is usually treated as such, but contrary to the behaviour of genuine Mode II crack it does not kink. Secondly, it is the existence and in-plane propagation of Mode I anti-cracks, which are the cracks that propagate under compressive load applied normally to their surface. In this case the load has the sign reverse to the conventional Mode I cracks giving the name to this type of cracks. They are observed in rocks and rock masses as compaction bands (e.g. [4-8]) and in laboratory experiments on rock samples in uniaxial compression as anti-wing cracks generated at the locations of compressive stress concentration created by pre-existing cracks [9, 10].

In-plane propagation of shear bands is usually associated with the formation of en-echelons of tensile (micro) cracks (e.g. [11-14]), however the process by which these cracks eventually merge and form the continuation of the shear band is not clear. Indeed, the tensile cracks grow parallel in the direction of maximum compressive stress. In order to merge the cracks should either start growing in a lateral direction, which is not possible, as they will be closed by the largest principal compressive stress, or to initiate shear microcracks by yet unknown mechanism. Thus even in the simple 2D case the mechanism of coalescence of en-echelon cracks is not clear. Even less clear is the mechanism of crack coalescence in 3D, when the orientation of the cracks forming en-echelon is more complex since they can rotate out of plane still being parallel to the direction of maximum compression.

Another challenge is to understand the mechanism of in-plane propagation of compaction bands and anti-wing cracks. For instance, the criterion of compaction band propagation cannot be based on simple substitution of rock failure in tension with rock failure in compression, as proposed e.g., in [15]. Indeed, the failure in compression is preceded by the formation of multitude of parallel tensile cracks in the direction of maximum compression (e.g., wing cracks). Such wing cracks are not observed in the compaction bands. On the contrary observations of thin sections suggest random orientations of cracks and grains within the compaction bands (e.g. [6, 16, 17]). Multiple microcracks are even observed in the directions normal to the direction of compression (see for instance the thin sections presented in [16]). Obviously, such microcracks cannot be produced by compressive stresses but it is conceivable that they are produced as a result of mutual rotations of the grains.

We *hypothesise* that both the compaction band and anti-wing crack propagation involves mutual rotation of the grains followed by fragmentation of the cement connecting the grains and subsequent rearrangement and compaction of the grains. (We note that the anti-wing cracks were observed in rocks with grain structure such as granodiorite, but never in homogeneous materials such as PMMA [10].) Given that grain rotations are directly observed in the shear bands in granular materials [18-20], we assume that grain rotations can also form the mechanism of in-plane shear band propagation.

Continuum modelling of rocks with grain rotations requires the use of Cosserat or micropolar continuum (e.g. [21-23]), which additionally considers rotational degrees of freedom and introduces the moment stress. Another difference from the classical continuum is that the Cosserat continuum possesses characteristic lengths (Cosserat characteristic lengths). Extensive research was devoted to cracks in such continua based on considering stress singularities at the crack tip, e.g. [24-27]. These singularities reflect the asymptotics of stress concentration when the distance to the crack tip tends to zero. In other words the traditional approach considers the distances smaller than the Cosserat characteristic lengths.

It was however pointed out in [29-31] that when a Cosserat continuum is used to model a particulate material such as rocks with grain microstructure, the asymptotics of small distances to the crack tip is beyond the resolution of the continuum. Indeed, a continuum description of a heterogeneous material is based on the introduction of representative volume elements whose size, H, is naturally much larger than the characteristic microstructural length, l_m, which is the scale at which the material can no longer be considered smooth. Then the equivalent continuum is introduced by averaging the relevant physical fields over these volume elements (e.g. [28]). While the equivalent continuum can formally address any distances, including infinitesimal, the interpretation of the calculated physical fields in terms of the original material (needed for instance to formulate the fracture criteria) is only possible in terms of distances *larger* than l_m. This concept poses no restrictions on classical continuum modelling since the classical continua are scale independent.

The situation however is different for higher order continua, such a Cosserat continuum, since they possess internal length scales. It was shown in [29-32] that for particulate materials in which particles are cemented to each other (e.g. rocks with granular structure or concrete), the Cosserat lengths are of the order of the grain size, l_m. Therefore the only asymptotics in the Cosserat continuum that are relevant to the particulate materials are the asymptotics that concern distances

$r >> l_m$. This translates into the notion that the meaningful Cosserat solutions are those that correspond to the asymptotics $r/l_m \to \infty$. We call such a continuum the *small-scale Cosserat continuum*. In this approach the relevant stress singularities at the crack tip are given by the intermediate asymptotics, which refers to the distances infinitesimal with respect to the crack dimensions but infinitely large compared to the Cosserat lengths. It is interesting that the technique of obtaining the intermediate asymptotics simplifies the analysis since the derivation of the asymptotics is less involved than the orthodox calculation of the stress singularities in Cosserat continuum.

In this paper we use the concept of the *small-scale Cosserat continuum* and propose a universal criterion of in-plane growth of shear cracks and compaction bands in compression based on the concentration of moment stresses. In this criterion the actual failure is produced by tensile fracturing of the cement layers between the grains caused by the bending moments associated with the concentration of moment stresses. This mechanism is independent of the sense of the moment stress; the latter only controls the location and direction of the induced tensile microcracks.

2. Crack propagation caused by moment stress concentration

The classical fracture criteria are based on the notion of crack propagation by separating two surfaces by applied stresses and expressing the conditions of the separation either in terms of critical forces or critical energy. In particulate materials consisting of particles (grains) and connected by cement bonds another micro failure mechanism can be at work: bending the cement layer by mutual rotation of adjacent particles and its cracking by flexure cracks, Fig. 1. Essentially what this mechanism is doing is translating the moment stress acting at scale H into microscopic tensile stresses at scale l_m. Since scale l_m is beyond the resolution of the (Cosserat) continuum that models the particulate material at scale $H >> l_m$, the failure criterion should be formulated in terms of moment stress μ_{ij}. Given that both stress and moment stress have singularity at the crack tip, we will use the approach proposed in [33] in which the crack propagation criterion is based on comparing the stress at a certain distance from the crack tip with the local material strength. It is natural to use l_m in place of such a length (see also [29-31]). Hence, for the simple case of fracture criterion controlled by a single moment stress component one has

$$\left|\mu_{ij}(l_m)\right| = \mu_c \,. \tag{1}$$

Here μ_{ij} is the moment stress component controlling local failure and the absolute value sign indicates that the instance of local failure is independent of the sense of the moment stress; the sign only controls the side of the link between the neighbouring particles from which it starts breaking. The critical value of moment stress μ_c represents the particular mechanism of bond breakage and microscopic properties of the material of the bond. From the symmetry analysis it can be found [29-31] that the moment stresses invoke the bond bending and fracturing shown in Fig. 2. It is seen that while the flexure cracks in Mode I crack are roughly coplanar with the main crack, the flexure cracks in Mode II crack form en-echelon of microcracks normal to the main crack. Yet, it is the bond (cement) breakage associated with relative particle rotations that separate the particles from the matrix and thus effect the crack propagation. The formation of en-echelon cracks is thus an accompanying phenomenon.

The proposed fracture criterion involves the use of the main terms of the double asymptotics $l_m/H \to 0$, $H/L \to 0$, where L is the characteristic length of the crack. The consistent application of this double asymptotics leads to the concept of small-scale Cosserat continuum.

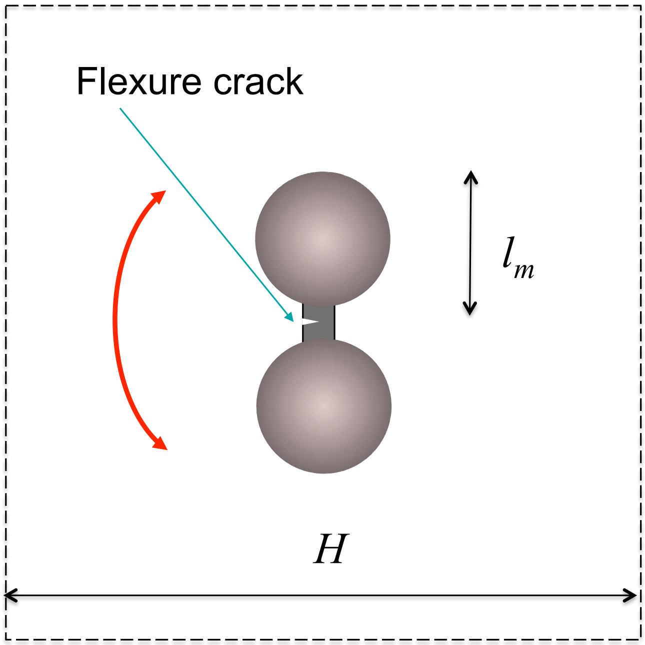

Figure 1. A volume element of size H loaded by a moment stress causing mutual rotation of neighbouring particles. The latter causes flexure (tensile) microcrack at scale l_m<<H.

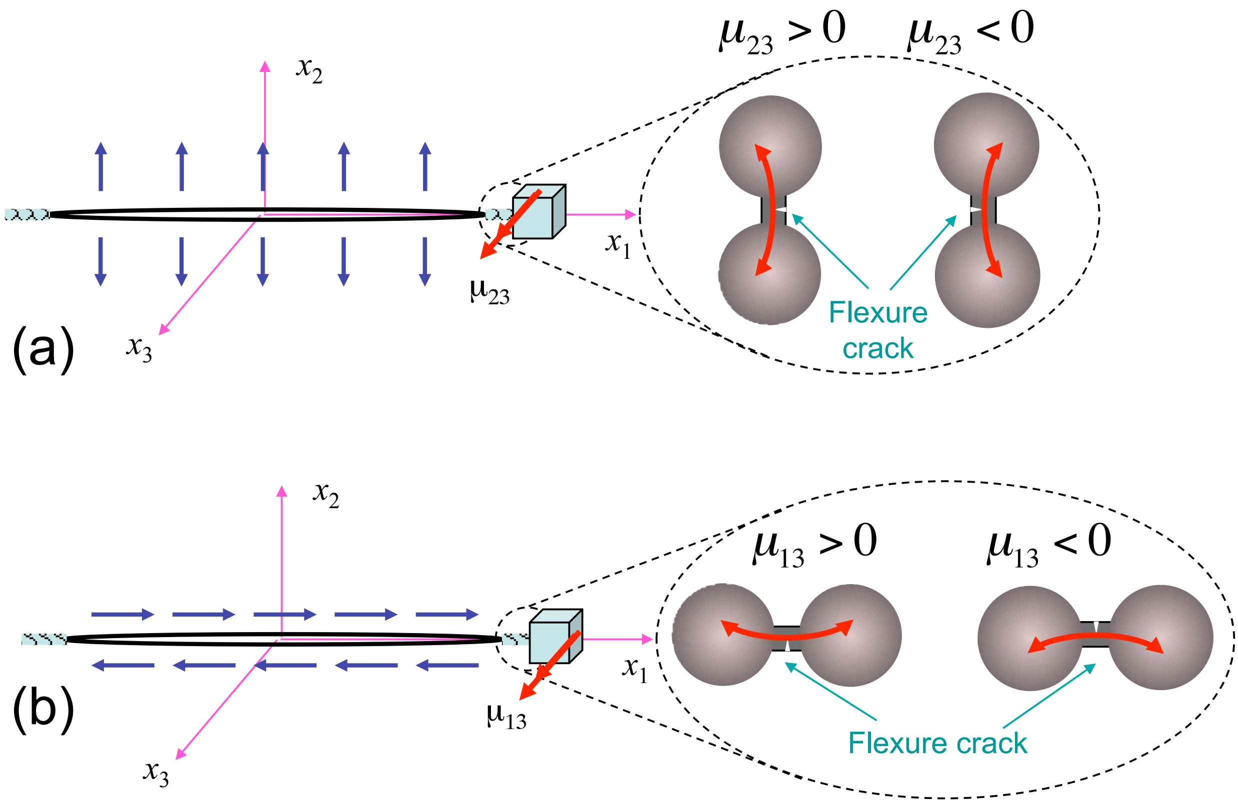

Figure 2. The direction of bending and the microcracking for (a) Mode I and (b) Mode II cracks. The corresponding bond is broken independently of the direction of microcrack (flexure crack) propagation, which is controlled by the sign of the corresponding moment stress.

3. Small-scale Cosserat continuum

We consider here the case of isotropic particulate material with internal rotations. The corresponding Cosserat continuum is defined by the following equilibrium and constitutive equations in the co-ordinate frame (x_1, x_2, x_3) (e.g. [34])

$$\sigma_{ji,j} = 0, \quad \mu_{ji,j} + \varepsilon_{ijk}\sigma_{jk} = 0, \quad i,j = 1,2,3$$
$$\sigma_{ji} = (\mu+\alpha)\gamma_{ji} + (\mu-\alpha)\gamma_{ij} + \lambda\gamma_{kk} \tag{2}$$
$$\mu_{ji} = (\gamma+\varepsilon)\kappa_{ji} + (\gamma-\varepsilon)\kappa_{ij} + \beta\kappa_{kk}$$

where σ_{ij} and μ_{ij} are stress and moment stress, ε_{ijk} is the alternating tensor. Here we use the deformation measures - the strain and curvature-twist tensors

$$\gamma_{ji} = u_{i,j} - \varepsilon_{kji}\varphi_k, \qquad \kappa_{ji} = \varphi_{i,j} \tag{3}$$

where u_i and φ_i are independent displacement and rotation vectors respectively and index (,j) denotes differentiation with respect to x_j, μ, α, γ, ε, λ, β are the Cosserat elastic moduli.

According to [29-31] the main term in the asymptotics $l_m/H \to 0$ can formally be obtained from the equations of the Cosserat continuum with constrained rotations (the couple stress continuum), where rotations are no longer independent of the displacements, but are related in the usual fashion

$$\varphi_i = \tfrac{1}{2}\varepsilon_{ijk}u_{i,k}\,. \tag{4}$$

Thus, the small scale Cosserat continuum formally involves a simpler theory – the couple stress theory. Further simplification is achieved if we recall that cracks can be represented as continuous distributions of dislocations and disclinations [35-37]. If we are interested in Modes I and II only then it can be shown that it is sufficient to consider only dislocations.

The determination of stress field produced by a dislocation involves solving the equations in displacements and rotations (with boundary conditions set in displacements) with the subsequent determination of the strain measures (3) and stress and moment stress fields using the constitutive law (2). In order to solve the equations for dislocations we use the correspondence theorem [24, 38] that states that any solution of the Navier equations (equations of equilibrium in displacements) of classical elasticity (without moment stress) is also a solution of the corresponding equations of equilibrium in displacements in the couple-stress theory, away from singular points [24]. Therefore the main asymptotic term of the stress and moment stress fields produced by dislocations can be obtained from the classical elastic solutions for the dislocations with the subsequent use of (4) for the already calculated displacement field to find the constrained rotations, the deformation measures (3) and finally the stress and moment stress using the constitutive relations (2).

Since the cracks are considered as appropriate distributions of dislocations, the above framework can be applied to determine the stress and moment stress produced by the cracks in the asymptotics of small-scale Cosserat continuum. In particular, this procedure can be used to determine stress and moment stress singularities in the intermediate asymptotics shown in Fig. 1. The resulting equations are presented in the following section.

4. Intermediate asymptotics for moment stress singularity at the crack tip

We consider a 2D crack in the plane strain approximation and find the stress singularities on the line of crack continuation using the theory outlined in the previous section. For a Mode I crack we obtain

$$\sigma_{11}(r) = \sigma_{22}(r) = \frac{K_I}{\sqrt{2\pi r}}, \quad \sigma_{12}(r) = \sigma_{21}(r) = 0, \quad \mu_{13} = 0, \quad \mu_{23} = -\frac{K_I l_m^2 \alpha}{2\mu}\frac{3-2\nu}{r^{3/2}\sqrt{2\pi}} \tag{5}$$

For a crack of Mode II we obtained the following stress singularities

$$\sigma_{11}(r) = \sigma_{22}(r) = 0, \quad \sigma_{12}(r) = \sigma_{21}(r) = \frac{K_{II}}{\sqrt{2\pi r}}, \quad \mu_{13} = \frac{K_{II} l_m^2 \alpha}{2\mu}\frac{4(1-\nu)+3}{r^{3/2}\sqrt{2\pi}}, \quad \mu_{23} = 0 \tag{6}$$

We see that the stress at the crack tip has the conventional square root singularity, while the moment stresses has stronger (power 3/2) singularity. This power of the moment stress singularity was reported in [24, 26, 38].

It is also worth mentioning that the moment stress μ_{23} in Mode I crack has the sign opposite to the sign of K_I. Thus for the conventional Mode I crack the moment stress is negative: the flexure cracks grow in the direction of propagation of the main crack, Figs. 2a, 3a. In the case of anti-crack the direction of flexure crack growth is opposite to the direction of propagation of the main crack, Figs. 2a, 3b. We emphasise that the role of flexure cracks is to initiate the breakage of the cement bonds between the particles, while the ultimate fracture propagation is produced by further particle rotations and particle detachment form the bulk of the material.

The beginning of flexure crack propagation and the resulting bond breakage are controlled by microscopic tensile stress on the edge of the bond, which is caused by moment stress μ_{23}. The value of the microscopic tensile stress is determined by the Cosserat continuum stresses σ_{22} and μ_{23} acting at a point $r=l_m$ of the continuum. In other words this is a superposition of the tensile stress generated by bending (moment stress μ_{23}) and the normal stress σ_{22}. The latter is positive for Mode I cracks and negative for anti-cracks, Fig. 3.

It was shown in [29] for Mode II crack that the microscopic tensile stress created by bending can be an order of magnitude higher than the conventional stress applied to the bond. This makes the mechanism based on moment stress the main fracture growth mechanism.

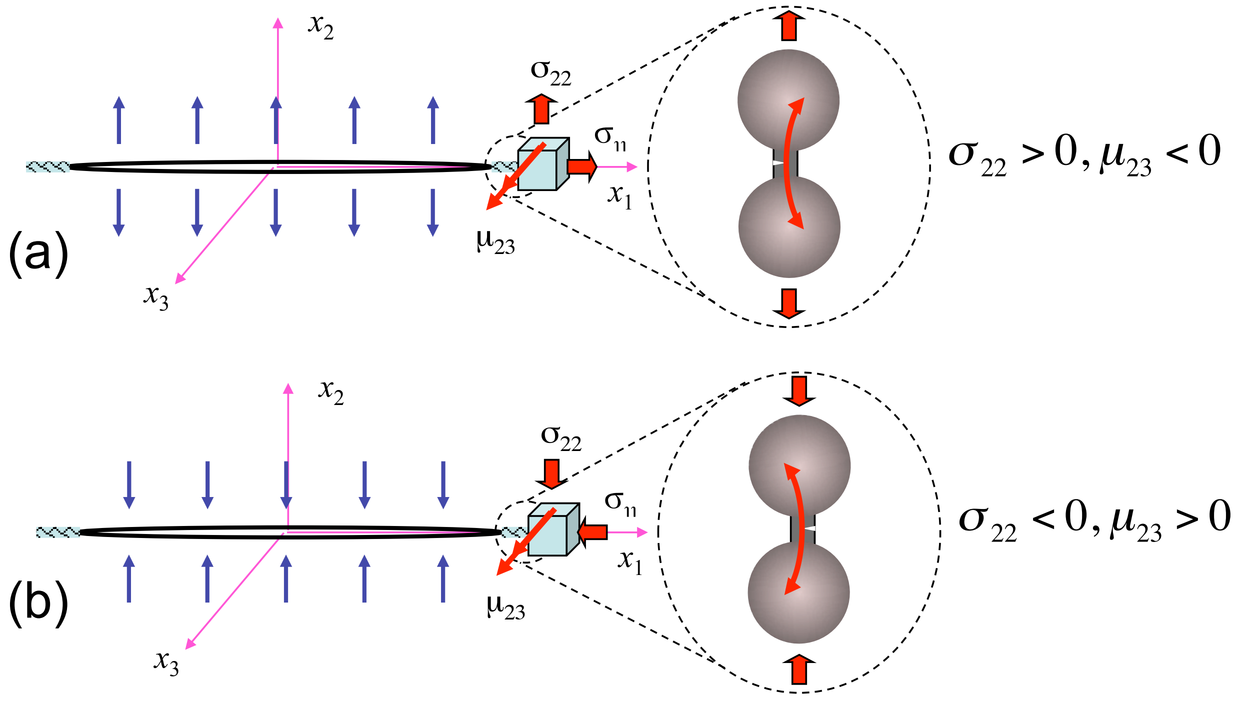

Figure 3. The directions of flexure crack propagation controlled by the sign of moment stress μ_{23}: (a) Mode I crack; (b) anti-crack.

5. Conclusions

Particulate materials such as rocks with granular microstructure and concrete permit relative rotations of the grains independent on their displacements. Therefore the criteria of crack propagation in such materials should include the grain (particle) rotations and the associated moment stresses. This is achieved by considering bending of the cement links/bonds between neighbouring particles caused by their relative rotation. The bending produces tensile stress on one side of the link, which eventually initiates a flexure crack (microcrack as seen from the scale of the propagating fracture). The initiation of the flexure crack leads to the link breakage and ultimately effects the particle detachment from the bulk of the material. The fracture mechanism based on link breakage and particle detachment is independent of the sign and source of the moment stress; only the side of the link where the flexural crack starts and the orientation/position of the link that is fractured first are affected. It is assumed that after the first link is broken the resistance to particle rotation is diminished sufficiently to permit breakage of other links and allow for the complete particle detachment. This criterion can explain the in-plane growth of Mode I and Mode II cracks as well as the anti-cracks (compaction bands).

Modelling of fracture propagation that involves moment stress requires the use of Cosserat (micropolar) continuum, which includes rotational degrees of freedom on top of the conventional translation ones. The Cosserat continuum possesses characteristic lengths that in the case of particulate materials with cement bonds/links between the particles are of the order of the particle size. Since the resolution of a continuum cannot be better than the microstructural length (the particle size in our case) the stress singularity at the crack tip only refers to the distances from the crack tip larger than the particle size and therefore larger than the Cosserat characteristic lengths. This leads to the concept of small-scale Cosserat continuum that is an asymptotics of small Cosserat lengths. This asymptotics formally leads to the Cosserat continuum with constrained rotations (the couple stress continuum). Modelling dislocations and Mode I and II cracks in such a continuum allows further simplification whereby the stress and moment stress distribution can directly be obtained from the displacement field produced by conventional dislocations and cracks by applying the relations of the couple stress theory. It was found that while the stresses have conventional square root singularity, the moment stresses have singularity of the power 3/2.

The actual fracture criterion is based on the stress and moment stress computed at a distance from the crack tip equal to the particle size (the Cosserat length). The tensile stress produced in the link/bond between particles by the moment stress is an order of magnitude higher than the one associated with the classical stress singularity. This suggests that the rotational mechanism of crack growth can actually supersede the traditionally perceived mechanism based on the tensile stress concentration only.

The flexure cracks formed in the process of particle rotations are seen at the scale of the crack as microcracks which are either coplanar to the main crack in the cases of Mode I crack or anti-crack or form en-echelon in the case of Mode II crack. The actual crack propagation is however caused by detachment (separation) of the particles from the bulk of the material and hence the appearance of en-echelon cracks is essentially a secondary effect accompanying the rotational mechanism of crack propagation.

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