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A MICRO-PROBABILISTIC APPROACH TO THE DUCTILE DEFORMATION AND FRACTURE OF METALS - I. PRELIMINARY INVESTIGATION

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INTRODUCTION

The conventional approach to the problem of deformation and fracture of metals is usually based on models which disregard the existing microstructure of the material. In this aspect, continuum and modified continuum models have been developed. These models are deterministic by definition and imply, within the restrictions of continuum mechanics, that all the basic quantities involved in the deformation process are continuous variables or functions of such variables which have, at least, continuous first order derivatives. Due to the existence of defects in the material and when these defects become significant, the field quantities fail to be continuous at the separating boundaries. Thus, it becomes necessary to consider these local effects as an integral part of the problem and to study the nature in detail, particularly in relation to the deformation process of the material system.

The present approach has been mainly aimed at formulating the deformation process in materials with strain history and having a discrete, and defective, microstructure. For this reason, the relevant field quantities characterizing either the geometrical or physical properties of the microstructure have been considered from the onset as random variables or functions of such variables [1, 2, 3]. The approach follows the concepts of the micromechanics theory of structural media due to Axelrad [1, 3].

Throughout the analysis, vector and second order tensor valued quantities may carry ~ or ≈ sign under the symbol respectively. However, third and fourth order tensors may be respectively indicated by ≋ and ≈≈ under the symbol.

LOCAL RESPONSE BEHAVIOUR

In order to describe the mechanical response of a medium which has a discrete microstructure, it is necessary to consider the local response behaviour which can differ considerably from the macroscopic response considered by phenomenological models. An element of the medium is defined as the smallest region of the microstructure that represents the mechanical and physical properties of the material at the microlevel. This element is chosen arbitrarily to represent the response behaviour of an individual grain (with the probability that the grain can be continuous or defective), as well as the bonding response within the grain boundary of the two matching grains. The latter is regarded, in the present stage of the analysis to be perfectly bonded.

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MS336

The deformation kinematics of an individual defective element "α" is shown in Figure 1. Denoting the incremental continuous displacement within the grain by $\Delta^\alpha U_i$, the incremental extension of the tip of the crack by $\Delta^\alpha C_i$ and the incremental deformation of the binding within the grain boundary between grains "α" and "β" by $\Delta^{\alpha\beta}d_k$. The overall incremental displacement within the element can be written:

$$\Delta^\alpha \omega_I = {}^\alpha\Lambda_{iI}(1-{}^\alpha\kappa)(\Delta^\alpha C_i + \Delta^\alpha U_i) + {}^{\alpha\beta}\Lambda_{kI}\;{}^\alpha\kappa\;\Delta^{\alpha\beta}d_k \;, \qquad (1)$$

where,

${}^\alpha\Lambda_{iI}$ = denotes the transformation from the grain coordinate frame ${}^\alpha y_i$ to the external frame Z_I.

${}^{\alpha\beta}\Lambda_{kI}$ = denotes the transformation from the grain boundary frame ${}^{\alpha\beta}x_k$ to the external coordinate frame Z_I,

and the parameter ${}^\alpha\kappa$, $0 \leq {}^\alpha\kappa \leq 1$, has been introduced to account for relative geometrical contribution of the grain to that of the grain boundary.

Although equation (1) expresses the overall incremental deformation of a defective grain in a general form, we differentiate in the analysis between the two following cases:

(i) the single grain is continuous, hence $\Delta^\alpha C_i = 0$

(ii) the single grain is defective by the existence of a sharp crack. Thus, the crack growth increment is predominant, i.e., $\Delta^\alpha C_i >> \Delta^\alpha U_i$ and $\Delta^\alpha U_i$ may be neglected.

Introducing now the probability that "α" is continuous, say ${}^\alpha p_1$, and the probability ${}^\alpha p_2$ that the same element is defective, one may express the overall incremental displacement within "α" in terms of probability in the following form:

$$\left.\begin{aligned} \Delta^\alpha \omega_I &= (1-{}^\alpha\kappa)[{}^\alpha p_1\;{}^\alpha\Lambda_{iI}\;\Delta^\alpha U_i + {}^\alpha p_2\,{}^\alpha\Lambda_{jI}\;\Delta^\alpha C_j] + {}^{\alpha\beta}\Lambda_{kI}\;{}^\alpha\kappa\;\Delta^{\alpha\beta}d_k \;, \\ {}^\alpha p_2 &= 1 - {}^\alpha p_1 \;, \end{aligned}\right\} \qquad (2)$$

where the transformation matrix ${}^\alpha\Lambda_{jI}$ indicates the orientation of the crack coordinate frame ${}^\alpha x_j$ with respect to the external frame Z_I as shown in Figure 1. The definition of the probability ${}^\alpha p_1$ and, hence, the probability ${}^\alpha p_2$ will follow subsequently in Section 3. In order to establish, however, the form of constitutive relation corresponding to (2) we consider first the incremental displacement $\Delta^\alpha U_i$.

Continuous Grain

The strain will be taken for simplicity as a linear one, thus, the strain increment within the grain can be expressed as:

$$\Delta^\alpha \underset{\approx}{\varepsilon} : \Delta^\alpha \varepsilon_{k\ell} = {}^\alpha\underset{\approx}{\nabla}\,(\Delta^\alpha \underset{\sim}{U}) \qquad (3)$$

where ${}^\alpha\underset{\approx}{\nabla}$ is the Tonti-Operator [4] and $\Delta^\alpha\underset{\approx}{\varepsilon}$ is regarded to be given by:

$$\Delta^\alpha\underset{\approx}{\varepsilon} = \Delta^\alpha\underset{\approx}{\varepsilon}^{(e)} + \Delta^\alpha\underset{\approx}{\varepsilon}^{(p)} \;. \qquad (4)$$

The plastic strain increment is assumed to be given by the flow rule as:

$$\Delta\varepsilon_{ij}^{(p)} = T_{ij}\;\Delta\;\lambda,\; T_{ij} = \partial f/\partial\xi_{ij} \qquad (5)$$

in which ξ_{ij} is the stress tensor, f is the yield function and $\Delta\lambda$ is a scalar function. The yield function is assumed to be given by the plastic work $W^{(p)}$, i.e.,

$$f(\xi_{ij}, \varepsilon_{ij}^{(p)}) = F(W^{(p)}) \;. \qquad (6)$$

Assuming a linear incremental constitutive equation then,

$$\Delta^\alpha\underset{\approx}{\xi} : \Delta^\alpha\xi_{ij} = {}^\alpha A_{ijk\ell}\;\Delta^\alpha\varepsilon_{k\ell} = {}^\alpha\underset{=}{A}\;{}^\alpha\underset{\approx}{\nabla}\;(\Delta^\alpha\underset{\sim}{U}) \;. \qquad (7a)$$

The following expression for the matrix $A_{ijk\ell}$ can be derived [2, 5]

$$A_{ijk\ell} = E_{ijk\ell} - 2\mu\;\xi'_{ij}\;\xi'_{k\ell}/\tfrac{2}{3}\,\bar{\xi}^2\;(F'/2\mu + 1) \;, \qquad (7b)$$

where $F' = \dfrac{\partial F}{\partial W^{(p)}}$, μ = shear modulus and $E_{ijk\ell}$ = elastic tensor modulus.

In arriving at (7b) the von Mises yield function has been assumed, i.e.,

$$f = \frac{1}{2}\,\xi'_{ij}\;\xi'_{ij} = \frac{1}{3}\,\bar{\xi}^2 \;. \qquad (8)$$

Grain Boundary

So far as the bonding effects, between the grains "α" and "β", are concerned, the most suitable form can be expressed in terms of a Morse function [6]. The analytical form of this function which will represent the 3-dimensional case can be written as follows:

$$ {}^{\alpha\beta}\psi = {}^{\alpha\beta}\psi_o\{\exp(-2b\,|{}^{\alpha\beta}\mathbf{d}|) - 2\exp(-b\,|{}^{\alpha\beta}\mathbf{d}|)\}\,, \qquad (9) $$

in which ${}^{\alpha\beta}\psi_o$ is the equilibrium interaction potential, b is the Morse constant and ${}^{\alpha\beta}\mathbf{d}$ is the deformation in the bond. An expression for the interaction incremental stress can be formulated as follows:

$$ \Delta^{\alpha\beta}\boldsymbol{\xi} = {}^{\alpha\beta}\mathbf{B}\;\Delta^{\alpha\beta}\mathbf{d}\,, \qquad (10) $$

where ${}^{\alpha\beta}\mathbf{B}$ is a material tensor operator for the bonding interaction which takes the form [2, 3]

$$ {}^{\alpha\beta}\mathbf{B} = \left[\frac{-2b^2\,{}^{\alpha\beta}\psi_o}{{}^{\alpha\beta}a}\;{}^{\alpha\beta}\mathbf{n}\;{}^{\alpha\beta}\mathbf{k}\;{}^{\alpha\beta}\mathbf{k}^{-1}\right], \qquad (11) $$

where ${}^{\alpha\beta}a$ = area per bond, ${}^{\alpha\beta}\mathbf{n}$ = outward unit normal to ${}^{\alpha\beta}a$, and ${}^{\alpha\beta}\mathbf{k}$ is a unit base vector associated with the local co-ordinate frame in Figure 1.

Defective Grain

The presentation of the relation between crack extension increment $\Delta^{\alpha}\mathbf{c}$, original crack length ${}^{\alpha}\mathbf{c}$ and the variation of the microstress within the individual grain, i.e., $\Delta^{\alpha}\boldsymbol{\xi}$, is based on the work of references 7, 8 and 9. The kinematics of crack growth are shown in Figure 2. In reference 9 to avoid the problem of a strain infinity at the crack tip, a fracture criterion was based on an average strain spread over a very small region of radius $|\boldsymbol{\varrho}|$ ahead of the crack. The latter may be referred to as a unit distance ahead of the crack tip, i.e., $|\boldsymbol{\varrho}| = 1$, with the understanding that this unit distance is very small compared to the grain size or even in comparison with the crack length. In order to express the building up of the strain history at an arbitrary point, say at a unit distance $|\boldsymbol{\varrho}| = 1$ from the tip, one has to consider the strain gradient caused by the variation of the local stress during the crack growth. To this effect, the gradient of the microstrain, obtained when the crack has reached to within one unit distance of the point in question, may be specified by both the local coordinates of the point, i.e., $\mathbf{y}$, and the current length of the crack $|\mathbf{c}|$. The gradient of microstrain has been building up ever since the plastic strain first swept over the point in question and may be described by [2, 8],

$$ \left(\frac{\partial^{\alpha}\boldsymbol{\varepsilon}(\mathbf{y},|\mathbf{c}|)}{\partial^{\alpha}\mathbf{y}}\right)_{|{}^{\alpha}\mathbf{c}|} = \left(\frac{\partial^{\alpha}\boldsymbol{\varepsilon}\;(\mathbf{y},|\mathbf{c}|)}{\partial^{\alpha}\mathbf{y}}\right)_{|{}^{\alpha}\mathbf{C}|} + \int_{|{}^{\alpha}\mathbf{C}|}^{|{}^{\alpha}\mathbf{c}|}\left[\frac{\partial}{\partial^{\alpha}\mathbf{y}}\left(\frac{\partial^{\alpha}\boldsymbol{\varepsilon}\;(\mathbf{y},|\boldsymbol{\eta}|)}{\partial\boldsymbol{\eta}}\right) + \frac{\partial}{\partial^{\alpha}\mathbf{y}}\left(\frac{\partial^{\alpha}\boldsymbol{\varepsilon}(\boldsymbol{\xi})}{\partial\boldsymbol{\xi}}\right)\frac{d^{\alpha}\boldsymbol{\xi}(|\boldsymbol{\eta}|)}{d|\boldsymbol{\eta}|}\right] d|\boldsymbol{\eta}|\,, \qquad (12) $$

in which $\boldsymbol{\eta}$ indicates the crack length variable*. The solution of (12) however, will be based on expressions for the microstress and microstrain in terms of the geometry of the crack and local coordinates. This solution may be written in an operational form as,

$$ \Delta^{\alpha}\mathbf{C} = {}^{\alpha}\boldsymbol{\Pi}(\boldsymbol{\xi})\Delta^{\alpha}\boldsymbol{\xi}\,. \qquad (13) $$

Constitutive Relation for the Structural Element

In view of equations (2), (7a), (10) and (13), one can write the response relation of a structural element in the following operational form:

$$ \Delta^{\alpha}\boldsymbol{\omega} = [(1-{}^{\alpha}\kappa)\{{}^{\alpha}P_1\;{}^{\alpha}\boldsymbol{\Lambda}\;{}^{\alpha}\mathbf{A}^{-1}(\boldsymbol{\xi}) + (1-{}^{\alpha}P_1)\,{}^{\alpha}\boldsymbol{\Lambda}\;{}^{\alpha}\boldsymbol{\Pi}\;(\boldsymbol{\xi})\} + {}^{\alpha\beta}\boldsymbol{\Lambda}\;{}^{\alpha}\kappa\,{}^{\alpha\beta}K\,{}^{\alpha\beta}\mathbf{B}^{-1}]\Delta^{\alpha}\boldsymbol{\xi}\,, $$

$$ = {}^{\alpha}\boldsymbol{\Gamma}\;(\boldsymbol{\xi})\;\Delta^{\alpha}\boldsymbol{\xi}\,. \qquad (14) $$

Note,

$$ \Delta^{\alpha\beta}\xi_{ij} = {}^{\alpha\beta}K\;\Delta^{\alpha}\xi_{ij}\,, \qquad (15) $$

where ${}^{\alpha\beta}K$ is an effective binding ratio [3].

The response equation (14) may be, also, written explicitly in terms of the stress increment as:

$$ \Delta^{\alpha}\boldsymbol{\xi} = {}^{\alpha}\boldsymbol{\Gamma}^{-1}(\boldsymbol{\xi})\Delta^{\alpha}\boldsymbol{\omega}\,, \qquad (16) $$

where in (14) and (16) ${}^{\alpha}\boldsymbol{\Gamma}\;(\boldsymbol{\xi})$ may be referred to as the material operator for the structural element [3, 10].

TRANSITION TO THE MACROSCOPIC RESPONSE BEHAVIOUR

Since the material system that occupies a given physical domain is regarded in the present approach as a discrete medium, a transition from the discrete description to the macroscopic one must be attempted. The concept of an intermediate domain between the microdomain and the macrodomain is introduced and specified by the requirements mentioned in [3, 10]. The choice of the intermediate domain is generally guided by the geometrical properties of the microstructure, as well as the boundary conditions imposed on the material specimen. In the case of a two-dimensional model of the material under uniaxial loading in the Z_1 direction, as shown in

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* As represented by the first term on the RHS of equation (12), there is an initial strain gradient at this point when crack starts to grow, i.e., at $|\mathbf{c}| = |\mathbf{C}|$. Then, the gradient is increased further by the strain occurring during crack growth. This is represented by the first term under the integral sign in equation (12). The second term represents a further increase in the strain gradient due to any change of the microstress within the grain, i.e., ${}^{\alpha}\boldsymbol{\xi}$.

Figure 3, the intermediate domain "M" can be arbitrarily specified by the region bound by two theoretical scanninglines $S_1 - S_1$, $S_2 - S_2$, perpendicular to the direction of loading. The width "μ" of such an intermediate domain "M", in the direction of the load, is determined by the requirement that this domain must contain a statistical number of elements α and, hence, statistical principles can be applied. One may establish, for instance, the internal distributions of the microdeformations and the microstresses. Letting ${}^{M}P\{\Delta\omega_I\}$ represents the probability distribution of a component of the incremental displacement vector $\Delta{}^{\alpha}\omega_I$ over an intermediate domain "M", then the mean value of this distribution can be written as:

$$
{}^{M}\langle\Delta\underset{\sim}{\omega}\rangle : {}^{M}\langle\Delta\omega_{\bar{I}}\rangle = \Sigma\ \Delta{}^{\alpha}\omega_{\bar{I}}\ \Delta{}^{M}P\ \{\Delta\omega_{\bar{I}}\}\ , \tag{17}
$$

where no summation over I is intended in the above, and the sequal given by an overbar. Referring to equation (14), one can also write the expression for ${}^{M}\langle\Delta\underset{\sim}{\omega}\rangle$, in general, as:

$$
\begin{aligned}
{}^{M}\langle\Delta\underset{\sim}{\omega}\rangle &= {}^{M}\langle\ \underset{\approx}{\Gamma}\ (\underset{\approx}{\xi})\Delta\underset{\approx}{\xi}\rangle\ , \\
&= {}^{M}\langle[(1-{}^{\alpha}\kappa)\{{}^{\alpha}P_1\ {}^{\alpha}\underset{\approx}{\Lambda}{}^{\alpha}\underset{\approx}{A}^{-1}(\underset{\approx}{\xi}) + (1-{}^{\alpha}P_1){}^{\alpha}\underset{\approx}{\Lambda}\ {}^{\alpha}\underset{\approx}{\Pi}\ (\underset{\approx}{\xi})\} + \\
&\quad + {}^{\alpha\beta}\underset{\approx}{\Lambda}\ {}^{\alpha}\kappa\ {}^{\alpha\beta}K\ {}^{\alpha\beta}\underset{\approx}{\beta}^{-1}]\ \Delta{}^{\alpha}\underset{\approx}{\xi}\rangle\ .
\end{aligned} \tag{18}
$$

The variance of the distribution of microdeformations can, however, be expressed by incorporating the fluctuating portion of $\Delta{}^{\alpha}\omega_{\bar{I}}$, i.e.,

$$
{}^{M}\langle\Delta\overset{*}{\omega}_{\bar{I}}\Delta\overset{*}{\omega}_{\bar{I}}\rangle = \Sigma\ (\Delta{}^{\alpha}\omega_{\bar{I}} - {}^{M}\langle\Delta\omega_{\bar{I}}\rangle)^2\Delta{}^{M}P\{\Delta\omega_{\bar{I}}\}\ ,
$$

and

$$
\Delta\overset{*}{\omega}_{\bar{I}} = \Delta{}^{\alpha}\omega_{\bar{I}} - {}^{M}\langle\Delta\omega_{\bar{I}}\rangle\ . \tag{19}
$$

With reference to the stress-deformation equation (16) for the structural element, the expression for the average value of the stress distribution within the intermediate domain may be written as:

$$
\begin{aligned}
\Delta{}^{M}\underset{\approx}{\sigma} &= {}^{M}\langle\ \underset{\approx}{\Gamma}^{-1}(\underset{\approx}{\xi})\ \Delta\underset{\sim}{\omega}\rangle\ , \\
&= {}^{M}\langle[(1-{}^{\alpha}\kappa)\{{}^{\alpha}P_1\ {}^{\alpha}\underset{\approx}{\Lambda}\ {}^{\alpha}\underset{\approx}{A}^{-1}(\underset{\approx}{\xi}) + (1-{}^{\alpha}P){}^{\alpha}\underset{\approx}{\Lambda}\ {}^{\alpha}\underset{\approx}{\Pi}\ (\underset{\approx}{\xi})\} + {}^{\alpha\beta}\underset{\approx}{\Lambda}{}^{\alpha}\ {}^{\alpha\beta}K{}^{\alpha\beta}\underset{\approx}{B}^{-1}]^{-1}\Delta{}^{\alpha}\underset{\sim}{\omega}\rangle
\end{aligned} \tag{20}
$$

and the variance of the internal stress distribution can be expressed by:

$$
{}^{M}\langle\Delta\ \overset{*}{\xi}_{\overline{IJ}}\ \Delta\ \overset{*}{\xi}_{\overline{IJ}}\rangle = \Sigma\ (\Delta\ \xi_{\overline{IJ}} - \Delta{}^{M}\sigma_{\overline{IJ}})^2\Delta{}^{M}P(\Delta\ \xi_{\overline{IJ}})\ ,
$$

and

$$
\Delta{}^{\alpha}\ \overset{*}{\xi}_{\overline{IJ}} = \Delta{}^{\alpha}\xi_{\overline{IJ}} - \Delta{}^{M}\sigma_{\overline{IJ}}\ . \tag{21}
$$

In the scheme of numerical evaluation of the above formulations, the above analysis is reduced to the case of pure shear within the structural elements of the microstructure. The choice of the case of pure shear is primarily due to that the solution of (12) and, hence, the form of the operator ${}^{\alpha}\underset{\approx}{\Pi}\ (\underset{\approx}{\xi})$ in equation (13) is obtainable [7, 8] in the case of pure shear.

For purpose of incorporating experimental measurements of microdeformations and in order to establish the connection [2, 3] between these measurements and the macroscopic values, i.e., equations (20) and (21), the surface of the intermediate domain may be subdivided into scanning areas. $A(A = 1, 2, \ldots, n)$ as shown in Figure 3. The size of each scanning area may be taken as $(\mu \times \mu)$. The definition of the scanning area within the intermediate domain serves further in defining a void ratio ${}^{A}p$ in this area. The latter may be taken as;

$$
{}^{A}P = a/A\ , \tag{22}
$$

in which "a" is the area of cracks or voids within A. Referring to the above formulations, it is assumed in the analysis that:

$$
P_1 = 1 - {}^{A}P\ . \tag{23}
$$

CONCLUDING REMARKS

The purpose of this paper has been to provide a general formulation for the deformation process in materials where the microstructure is treated as being discrete by including the probability of cracks or flaws to exist within the material. A three dimensional analysis has been presented which can be applied in principle, to a wide class of "defective" ductile materials. However, it is recognized that a rigorous evaluation of various quantities in the analysis will often prove impossible if predictions are to be made for real materials, with complex microstructures, subjected to multi-axial loading. However, it is believed the work offers some suggestions for accounting for the influence of certain structural features of a material on the deformation and fracture process.

In the first instance some simple experiments could be conducted to test out the theoretical model. For example, one could look at the influence of a controlled but varying, grain size on the response of a specimen under uniaxial and biaxial loading conditions.

On the basis of the present approach it is also suggested that the analysis could be extended to include,

(i) Probable effects of failure or breakage of the binding within the grain boundaries. Thus, a correlation between the progression of failure of the grain and that in the grain boundary may be established.

(ii) Space and time evolutions of the distribution of internal microdeformations and, hence, the evolution of the corresponding distribution of internal stresses. Hency by specifying, for instance, a limit of deformation within the individual structural elements, it may be possible to establish a fracture criterion within the intermediate domain. Considering that the macroscopic specimen contains an innumerable number of non-intersecting intermediate domains, [1, 3, 10] the location of earliest fracture site of the specimen may be predicted.

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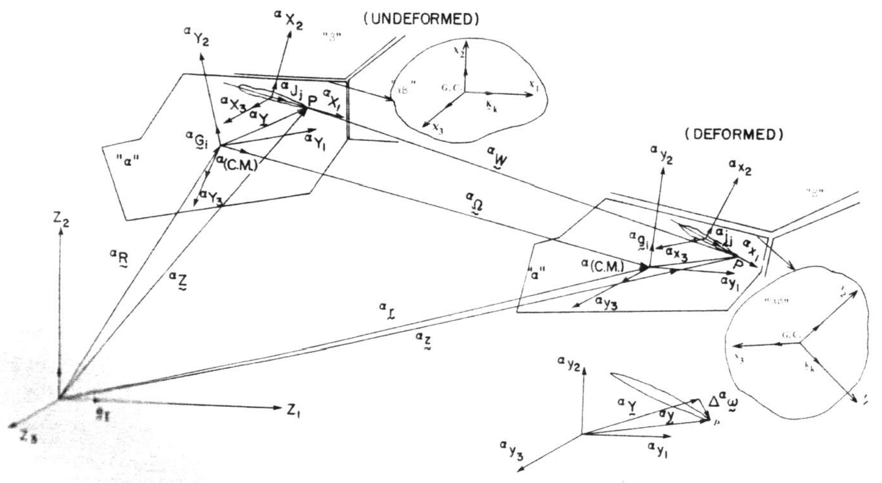

Figure 1 Deformation Kinematics of an Individual "Defective" Structural Element "α"

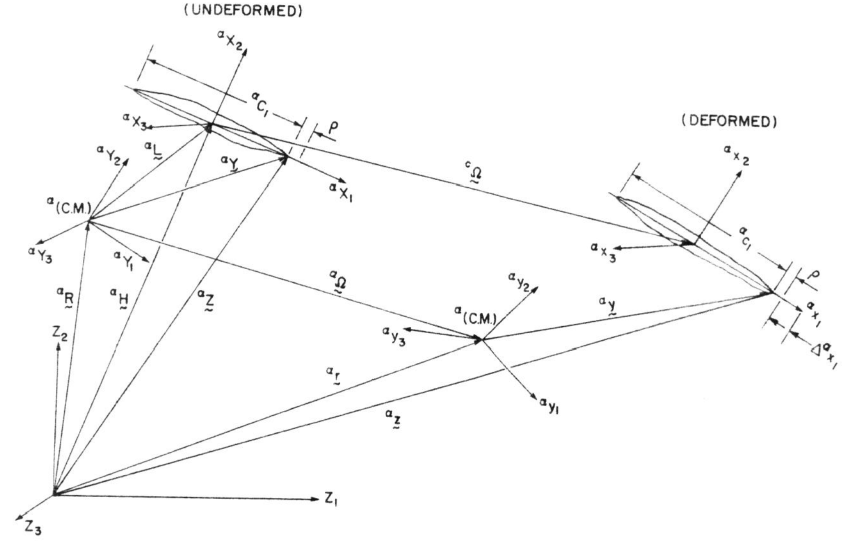

Figure 2 Kinematics of Crack Growth in an Element "α"

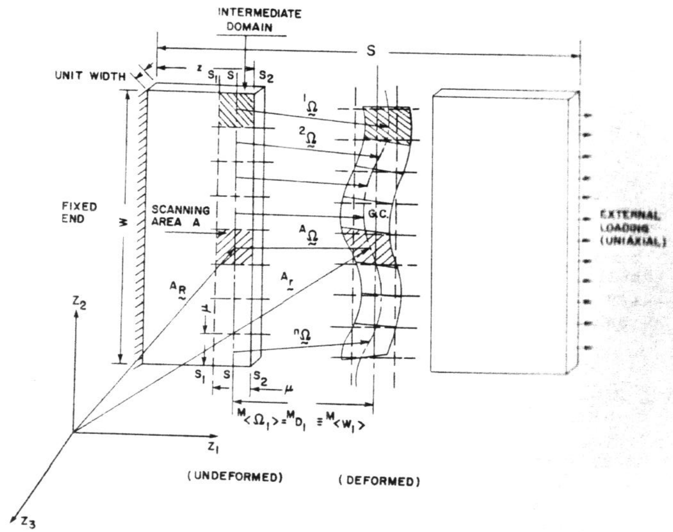

Figure 3 The Concept of the Intermediate Domain in the Macroscopic Specimen