Int. J. Solids Structures Vol. 30, No. 15, pp. 2097–2108, 1993
Printed in Great Britain

0020–7683/93 $6.00+.00

A UNIVERSAL PHYSICALLY CONSISTENT DEFINITION OF MATERIAL DAMAGE

C. W. Woo and D. L. Li
Department of Mechanical Engineering, University of Hong Kong, Pokfulam Road, Hong Kong

(*Received* 1 *April* 1992; *in revised form* 16 *February* 1993)

Abstract—This paper proposes a physically consistent definition of material damage. The definition is based on the physical concepts of inter-atomic energy and the breaking and re-establishing of the atomic bonds. The states of material damage are physically determined in a broad sense by the configuration of the atomic bonds. The meso characteristics, such as vacancies, dislocations, pores, slips, microcavities, microcracks and so on, could be quantified through the use of subsystems each corresponding to a special configuration. The constitutive equations, referring to the material damage represented by the definition, could be developed by following both nonlocal and local theories.

1. INTRODUCTION

It has been recognized in practice that the failure of most engineering components or structures follows a process of time and environment dependent damage. In the last few decades, researchers have been trying to develop theories and analytical models to elucidate the process quantitatively. These theories and models involve the use of different scale parameters to describe a wide range of physical characteristics including micro, meso and macro behaviors, and can be divided into nonlocal (strong or weak nonlocal) and local theories [see Kröner (1963, 1968) and Kunin (1975, 1982, 1983)].

For strong nonlocality or spatial dispersion, the corresponding theory compares physical wavelength with the scale parameter. In this case, the scale parameter may refer to a distance between particles in discrete structures or to grain size. It means that the physical and geometrical nature of the solid microstructure in the order of crystal lattice, vacancies or dislocations could be considered by the model. However because of the large number of such quantities involved in a solid, it is difficult to develop a closed-form mathematical solution. The statistical method, such as that used by quantum mechanics and statistical mechanics, should therefore be employed.

To reduce the difficulty in developing an analytical model and at the same time to retain partly the effects of nonlocality, a weakly nonlocal model in which the scale parameter is small in comparison with the wavelength of the solid considered could be suitable. It is an approximate model in comparison with the strong nonlocal model, for which integral and finite-difference operators are replaced by differential operators with small parameters attached to their highest derivatives. Several theories, such as multipolar, asymmetric, micromorphic and couple-stress theory [see e.g. Truesdell and Toupin (1960), Edelen *et al.* (1971), and Eringen (1978)] belong to this type, although they are usually constructed on a purely phenomenological basis.

By considering a sufficiently long wavelength (zeroth longwave approximation), the nonlocal model could be translated to a local theory, in which there are no scale parameters involved. It means that all characteristics of microstructure and mesostructure are smeared by an averaged or homogenized process. The property of locality, i.e. the possibility of considering "infinitesimally small" elements of the medium is inherent in all the classical theories of the continuum mechanics and macro continuum damage mechanics [see Lemaître (1987, 1992) and Chaboche (1988a, b)]. The transition from nonlocality to locality has made an enormous simplification in the mathematical analysis, leaving relatively simple mathematical expressions.

For practical purposes, one is interested in developing some theories with simple mathematical expressions, but having a certain degree of power to reflect the effects of

nonlocality. To do so, a possible approach is to bridge the physical concepts and mathematical expressions between the nonlocal and local theories. The difficulty in mathematical manipulation involving discrete media to be described by discrete functions could be overcome by introducing, for example, a concept of "quasicontinuum" [see Kunin (1983)]. In essence it is an interpolation of functions of discrete argument by a special class of analytical functions in such a way that the condition of one-to-one correspondence between quasicontinuum and the discrete medium is fulfilled. The example for the physical simplification is made by the so-called effective field theories, such as self-consisent theory. From the theory, the cells (slip plane, defect or crack, etc.) represented by scale parameters are considered to be embedded in isolation into a homogeneous medium which in some appropriately smeared sense reflects the influence of adjacent cells. These theories enable discrete and continuous media to be described within the scope of a unified formalism and to be generalized correctly in such concepts of continuum mechanics as strain and stress. However, when damage as an internal variable is introduced into the constitutive theory of material, confusion arises from the lack of a physically and geometrically consisent representation of damage. Accordingly, it is important to establish a physically and geometrically acceptable definition of damage, which is the purpose of this paper.

For a possible extension to all the scale parameters interested, it is obvious that the representation of damage should be related to a physical cell as small as possible, such as the size of an atom. In this paper, the bonds referring to the interaction of atoms as characteristic physical cells will be used to represent the material damage. As a preliminary study, it is appropriate to confine our attention to some simple situations. These simple situations include both the solid with simple microstructure and the damage with the simplest mathematical description, i.e. scalar.

2. BASIC CONCEPTS AND DEFINITION OF MATERIAL DAMAGE

By the 1920s, it was recognized that materials are much weaker than their theoretical strength calculated from a perfect crystalline material. It means that a certain degree of damage had existed before mechanically and environmentally induced damage. Therefore, it is reasonable to describe damage by considering the atomic structure of a solid.

According to the theory of quantum mechanics, atoms in condensed phases occupy equilibrium positions and are vibrating about the valley of the inter-atomic energy curve (see Fig. 1). When external work is applied, the atoms are displaced from their equilibrium

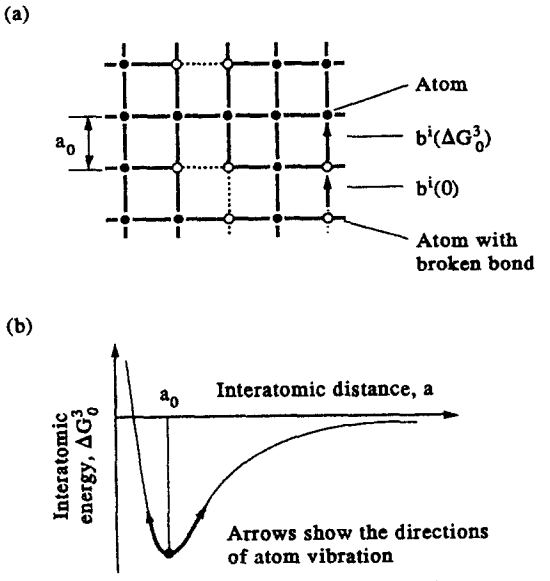

Fig. 1. (a) The configuration of atoms and bonds in a simple crystalline structure; (b) the interatomic energy versus distance between two atoms.

position and so the potential energy of the system is changed. If external work is generated by stress and the resulting deformation is elastic, the potential energy of the system is stored in a reversible manner. On the removal of the stress, the atoms move back to their equilibrium position, and the increase of the potential energy of the system is released. Superimposed on this reversible process is the time-dependent, thermally activated irreversible process. Under these conditions, the atoms overcome their energy barriers causing the breaking of the previous bonds and re-establishing new configuration of bonds, and move into a new equilibrium valley of free energy. In other words, irreversible microstructural alteration or damage occurred. It is this fundamental and general fact that the process of damage in crystalline materials and in polymers should be considered as a chemical reaction in which the composition remains constant but the bond structure of atoms changes. Accordingly, the thermodynamic theory of irreversible processes is suitable for the description of damage process as long as the internal variable D is defined rationally.

2.1. *System including* n *single atomic bonds*

Consider atoms moving in the "configuration space" as shown in Fig. 1, the bond between two atoms of a real material could be determined by an axial vector

$$\mathbf{b}^i(\Delta G^s) = b^i(\Delta G^s)\mathbf{L}_b^i, \quad (i = 1, 2, 3, \ldots, n), \tag{1}$$

with $b^i(0) = 0$, in which $\mathbf{L}_b^i$ is the characteristic direction vector and ΔG^s denotes the single inter-atomic energy. $b^i(\Delta G^s)$ indicates that the intensity of cohesion between two atoms is dependent on the inter-atomic energy, i.e. the physical and microstructural characteristics of the material and $b^i(0) = 0$ means that the ith bond has ceased to cohere two atoms.

With relation to $\mathbf{b}^i(\Delta G^s)$, the damage could be described in two ways: One is to take $\mathbf{b}^i(\Delta G^s)$ in comparison with $\mathbf{b}^i(\Delta G_0^s)$ as a measure of damage, in which ΔG_0^s denotes the inter-atomic energy of the perfect materials, and another is to take the number of the broken bonds, i.e. the number of bonds with $\mathbf{b}^i(0) = 0$, as a measure of damage. For the former, damage is based on the concept of inter-atomic energy which is characteristic of microstructure. In this case, the ideal or perfect state to be represented by $\mathbf{b}^i(\Delta G_0^s)$ could be taken as the reference background (no damage). Consequently, the scalar measure of solid damage D for the system including n atomic bonds is defined as the difference between the weighting sum of the inter-atomic energy of an ideal material and that of a practical one (non-dimensional over the weighting sum of the inter-atomic energy of an ideal material), i.e.

$$D = \frac{\sum_{i=1}^{n} (\mathbf{b}^i(\Delta G_0^s) - \mathbf{b}^i(\Delta G^s))\mathbf{N}}{\sum_{i=1}^{n} \mathbf{b}^i(\Delta G_0^s)\mathbf{N}} = 1 - \frac{\sum_{i=1}^{n} b^i(\Delta G^s)\mathbf{L}_b^i \cdot \mathbf{N}}{\sum_{i=1}^{n} b^i(\Delta G_0^s)\mathbf{L}_b^i \cdot \mathbf{N}}, \tag{2}$$

where the weighting function is the scalar product of the unit direction vector $\mathbf{L}_b^i$ of each bond and the unit normal vector $\mathbf{N}$ of the plane considered. Through the weighting function, the influence of the orientations of bonds on damage could be included. This definition might be useful in the qualitative or quantitative analysis of the damage of materials induced by the metallurgical or synthetic processes.

Another way, which may be more suitable for the description of mechanical damage, is to consider, as the measurement of material damage, whether the bond is broken or not. For this case, the scalar measurement of damage D in the plane of the material cell with unit normal vector $\mathbf{N}$ is defined as

$$D = \frac{\sum_{i=1}^{n} \mathrm{s}(\mathrm{b}^i(\Delta \mathrm{G}^s))\mathbf{L}_b^i \cdot \mathbf{N}}{\sum_{i=1}^{n} \mathbf{L}_b^i \cdot \mathbf{N}}, \tag{3}$$

in which n denotes the number of bonds through the plane considered and the selection function

$$s(b^i(\Delta G^s)) = \begin{cases} 1, & \text{when } b^i(\Delta G^s) = b^i(0) = 0 \\ 0, & \text{otherwise} \end{cases}, \quad (i = 1, 2, \ldots, n), \tag{4}$$

acts as a selector separating the broken bonds from the complete ones. $\mathbf{L}_b^i \cdot \mathbf{N}$ is the projection of the direction vector of bond along the normal direction of the plane considered, and acted as the variable of orientation of bonds on damage. If the characteristic area of the ith bond, defined as the area to be taken by a projection of the effective space of an atomic bond occupied in the system configuration space onto a plane with normal vector $\mathbf{L}_b^i$, is denoted as ϑ^i, the projective area of ϑ^i onto the plane with unit normal vector $\mathbf{N}$ is $\vartheta^i \mathbf{L}_b^i \cdot \mathbf{N}$ (see Fig. 2). Accordingly, the total area A of n atomic bonds crossing the plane is

$$A = \sum_{i=1}^{n} \vartheta^i \mathbf{L}_b^i \cdot \mathbf{N}. \tag{5}$$

If taking $\vartheta = \text{mean}(\vartheta^i) = \langle \vartheta^i \rangle$, $(i = 1, 2, \ldots, n)$, then

$$A = \vartheta \sum_{i=1}^{n} \mathbf{L}_b^i \cdot \mathbf{N}. \tag{6}$$

From eqn (6), the meaning of $\mathbf{L}_b^i \cdot \mathbf{N}$ is obvious.

The material damage defined by eqns (2) and (3) is based on a purely physical point of view. Almost no additional assumptions are attached to this definition. In addition, there exists no direct interaction among the atomic bonds as they are spatially separated in the solid. However, since a solid contains atomic masses of the order of 10^{24} per cm^3, the damage cannot be described by the usual analytical modeling through the consideration of the individual bond one by one. If the process of averaging in the statistical sense is adopted, the meso characteristics of the materials involved in the influences of vacancies, dislocations, pores, slips, microcavities, microcracks and so on will be buried completely. To avoid this, it is advisable to group the bonds according to their meso characteristics and then to consider these groups of bonds instead of considering the total bonds one by one. To do so, let us consider every group as a subsystem. The configuration of the system will be composed of the total configurations of the subsystems.

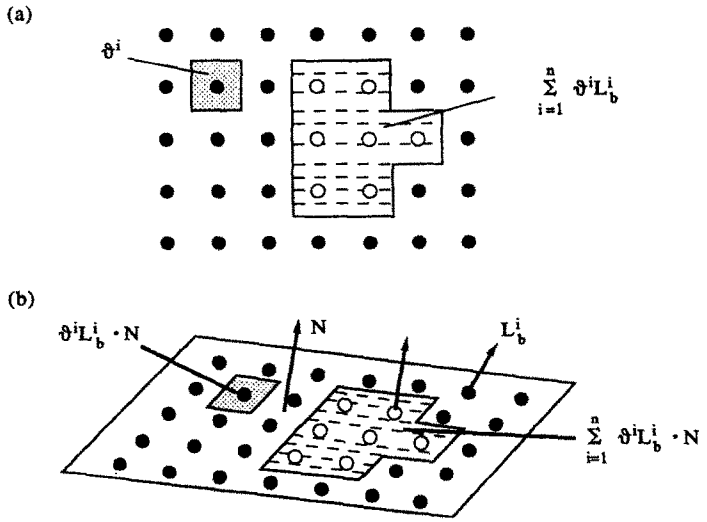

Fig. 2. (a) The characteristic area of bonds; (b) the projective area of ϑ^i on to the plane with unit normal vector $\mathbf{N}$.

2.2. *System including* m *subsystems*

Depending on the scale used, the subsystem could be generated in a number of ways. For example:

(a) by grouping together the bonds which are adjacent to each other and with same inter-atomic energy as a subsystem;
(b) by grouping together the bonds which are adjacent to each other and with same orientation as a subsystem;
(c) by grouping together the bonds with the same inter-atomic energy but distributed randomly in the whole system as a subsystem.

To sum up, for every subsystem there is a unique meso characteristic of solid. Damage in a cell in the plane of the material could be described by a system configuration composed of the configurations of these subsystems with bonds crossing through the plane. However, for practical considerations, the subsystem should be set up in a plane band with the characteristic thickness, say $2t$, rather than in a rigorous plane with zero thickness. Accordingly, m subsystems describing the meso characteristics of material in a plane cell with thickness $2t$ are determined by m vectorial functions

$$\mathbf{g}^i(\Delta G^g, \chi) = g^i(\Delta G^g, \chi)\mathbf{L}_g^i, \quad (i = 1, 2, \ldots, m), \tag{7}$$

where χ is a characteristic variable relating to the location of subsystems in the configuration space of system, $\mathbf{L}_g^i$ is the characteristic unit direction vector of the subsystem and ΔC^g denotes the free energy of the subsystem considered, from which the intensity of energy barrier is determined. When a subsystem is composed of a group of bonds to represent a part of the grain boundary of a polycrystalline solid, the energy barrier signifies the resistance to be overcome by the external work and $\mathbf{L}_g^i$ is the unit normal vector of the grain plane. If a subsystem is grouped by the special bonds with $\Delta G^s = 0$ to present a microcrack, ΔG^g is equal to zero and $\mathbf{L}_g^i$ denotes the unit normal vector of the microcrack plane.

Corresponding to the definition described in Section 2.1, the damage in the plane considered is defined as

$$D = \frac{\sum_{i=1}^{m} (\mathbf{g}^i(\Delta G_0^g, \chi) - \mathbf{g}^i(\Delta G^g, \chi))\mathbf{N}}{\sum_{i=1}^{m} \mathbf{g}^i(\Delta C_0^g, \chi)\mathbf{N}} = 1 - \frac{\sum_{i=1}^{m} g^i(\Delta G^g, \chi)\mathbf{L}_g^i \cdot \mathbf{N}}{\sum_{i=1}^{m} g^i(\Delta G_0^g, \chi)\mathbf{L}_g^i \cdot \mathbf{N}}, \tag{8}$$

and

$$D = \frac{\sum_{i=1}^{m} s(\mathbf{g}^i(\Delta G^g, \chi))\mathbf{L}_g^i \cdot \mathbf{N}}{\sum_{i=1}^{m} g_1^i(\chi)\mathbf{L}_g^i \cdot \mathbf{N}} = \frac{\sum_{i=1}^{m} s(\mathbf{g}^i(\Delta G^g, \chi))\mathbf{L}_g^i \cdot \mathbf{N}}{\sum_{i=1}^{n} \mathbf{L}_s^i \cdot \mathbf{N}}, \tag{9}$$

in which m denotes the number of subsystems in the plane cell with unit normal vector $\mathbf{N}$ and thickness $2t$. The selection function is defined as

$$s(g^i(\Delta G^g, \chi)) = \begin{Bmatrix} g_1^i(\chi), & \text{when } \Delta G^g = 0 \\ 0, & \text{otherwise} \end{Bmatrix}, \quad (i = 1, 2, \ldots, m), \tag{10}$$

in which $g_1^i(\chi)$ is a function of location which could be set to one regardless of location.

3. PROPERTIES OF THE PROPOSED DEFINITION

The material damage defined by eqns (2) and (8) is based on the physical concept of the inter-atomic energy of atomic bonds, which is characteristic of microstructures of solids. The ideal or perfect crystalline structure with active energy (or bond energy) ΔG_0^s is taken

as the reference point for the quantitative representation of material damage. It means that a certain degree of damage exists in all practical solids. The main advantage for doing so is that the damage caused by the metallurgical or synthetic processes of material could be represented quantitatively. As $b^i(\Delta G_0^s)$ is always equal to or larger than $b^i(\Delta G^s)$ and $b^i(\Delta G^s)$ is equal to or larger than zero for all i, the damage defined by eqns (2) and (8) always has a value between zero and one.

The damage defined by eqns (3) may be more suitable for the representation of material damage caused by the external loading and/or environments. The meso characteristics involving slip plane, microcavities, microcracks and so on could be conveniently described through the introduction of the concept of a subsystem expounded mathematically by eqn (9). It is obvious that the damage defined by eqns (3) and (9) also has a value between zero and one because some positive terms in the sum of numerators of these equations are omitted by the selection functions.

According to the proposed definition, the state of damage is determined only by the state of atomic bonds of the system considered. Any changes in the microstructures of the solid will contribute a certain ingredient to damage. It is not simply confining damage as the impairment of the stress transmitting capacity, although the impairment is possible as a result of the presence of microcracks resulting in some changes in microstructures. Damage as a change of internal structures of material should have a much wider meaning in physics. Any inelastic phenomena with or without reduction in material stiffness or strain softening could be described in a broad sense by the proposed definition.

In addition to its rigorous physical foundation which is an important factor for most of the damage theories, the definition could also provide a scheme to establish a geometrically consistent representation for different scale parameters. The scheme is based upon a subsystem model in the system configuration space of atomic bonds. Several simple examples are shown in the following three sections.

4. MICROMECHANICS OF MATERIAL DAMAGE

Consider a solid in which the nucleation and growth of microcracks is the only mode of irreversible changes in the microstructure. The solid was modeled by an arbitrary distribution of flat planar microcracks with the concentration being dilute enough to not create any significant overlap of projections. It assumes that these microcracks are surrounded by some homogenized effective medium which in some appropriately smeared sense reflects the influence of adjacent microcracks. The nonlinear responses of this solid have been studied quite well [see Krajcinovic (1985), Krajcinovic and Sumarac (1987) and Krajcinovic (1987)].

First, consider an elementary volume with a plane cell of area A to be crossed by n atomic bonds defined by eqn (1) as a system, which is large enough to contain a sufficient number of microcracks and still small enough to be mapped onto a material point. This system is composed by $m+1$ subsystems. Among $m+1$ subsystems, m are represented by

$$\mathbf{g}^i(\Delta G^g, \chi) = \left(\sum_{j=1}^{ni} \mathbf{L}_s^j \cdot \mathbf{L}_g^j \right) \mathbf{L}_g^i, \quad (i = 1, 2, \ldots, m), \tag{11}$$

where ni denotes the number of bonds for the ith subsystem crossing the plane with the unit normal vector $\mathbf{L}_g^i$. Obviously, the area of the ith microcrack to be represented by the ith subsystem is, in view of eqn (6),

$$\xi^i = \vartheta \sum_{j=1}^{ni} \mathbf{L}_s^j \cdot \mathbf{L}_g^i, \quad (i = 1, 2, \ldots, m). \tag{12}$$

The $(m+1)$th subsystem is represented by

$$\mathbf{g}^{m+1}(\Delta G^{g}, \chi) = \left(\sum_{i=1}^{n} \mathbf{L}_{b}^{i} \cdot \mathbf{N} - \sum_{j=1}^{m} \mathbf{g}^{j}(\Delta G^{g}, \chi) \cdot \mathbf{N} \right) \mathbf{N}. \tag{13}$$

According to eqn (9), damage can be described by

$$D = \frac{\sum_{i=1}^{m} s(\mathbf{g}^{i}(\Delta G^{g}, \chi)) \mathbf{L}_{g}^{i} \cdot \mathbf{N}}{\sum_{i=1}^{n} \mathbf{L}_{s}^{i} \cdot \mathbf{N}} = \frac{\sum_{i=1}^{m} \xi^{i} \mathbf{L}_{g}^{i} \cdot \mathbf{N}}{A}. \tag{14}$$

If $\mathbf{L}_{g}^{i} = \mathbf{L}_{g}$, for $i = 1$ to m, are parallel (i.e. system of parallel microcracks) and introducing the concepts of the "averaging variables" proposed by Krajcinovic (1985), the field of m parallel microcracks could be grouped by k axial vectors $\omega^{j}\mathbf{L}_{g}$ $(j = 1, 2, \ldots, k)$. Moreover, if the half characteristic thickness t equals the characteristic length l used by Krajcinovic (1985), then eqn (14) becomes

$$D = \frac{\sum_{i=1}^{m} \xi^{i} \mathbf{L}_{g}^{i} \cdot \mathbf{N}}{A} = \frac{\sum_{j=1}^{k} \bar{\xi}^{j} \mathbf{L}_{g} \cdot \mathbf{N}}{A} = \sum_{j=1}^{k} \omega^{j} \mathbf{L}_{g} \cdot \mathbf{N}, \tag{15}$$

in which $\bar{\xi}^{j}$ is the sum of microcrack areas within the band $(-l, l)$ corresponding to ω^{j}. This representation is the same as the one proposed by Krajcinovic (1985) and could be extended to a general microcrack field.

5. MACRO PHENOMENOLOGICAL THEORY

The macro phenomenological theory, alluring in its simplicity, is primarily focused on the macro events, i.e. average value in the statistical sense. Theoretically, in view of thermodynamics with internal variable method, the observed macro nonequilibrium state could be sufficiently well approximated by a constrained state of thermodynamic equilibrium corresponding to the current values of a finite set of internal variables [see Kestin and Rice (1970), Rice (1971), and Kestin and Bataille (1978)].

After introducing a macro damage variable D, as an internal variable, Damage Mechanics (DM) could be used to describe the effects of irreversible microstructural alterations on macroscopic mechanical properties of solids such as stiffness and strength. Since the pioneering works by Kachanov (1958) and Rabotnov (1963), the theory of DM has been quickly developed and evolved as a practical tool to model the damage processes of engineering material and structures at a macroscopic continuum level.

However, it seems that a physically and geometrically consistent definition of material damage has not appeared yet. Some confusions are found in the constitutive equations of the materials and a host of substantially different methods dealing with the same phenomenon have been spawned [see Krajcinovic (1984) and Rabier (1989)]. To enable the proposed physically consistent definition to be used as a macro internal variable to represent material damage, a system of atomic bonds composed of only one subsystem is taken to define the damage variable. Of course, the system will contain a full elementary volume which is defined as a material point in DM.

Considering a plane cell, with unit normal vector $\mathbf{N}$, crossing the elementary volume and assuming the characteristic area ϑ^{i} is the same for all n bonds crossing through the plane. From eqn (3), damage is defined as

$$D = \frac{\sum_{i=1}^{n} s(b^i(\Delta G^s))\mathbf{L}_b^i \cdot \mathbf{N}}{\sum_{i=1}^{n} \mathbf{L}_b^i \cdot \mathbf{N}} = \frac{\vartheta \sum_{i=1}^{n} s(b^i(\Delta G^s))\mathbf{L}_b^i \cdot \mathbf{N}}{A}. \tag{16}$$

where A is the overall cross-sectional area of the element considered and $s(b^i(\Delta G^s))$ is defined in eqn (4). If $\tilde{A}$ denotes the effective area to support the external load after damage caused by the presence of microcracks and microcavities, in view of eqn (6), then

$$\tilde{A} = A - \vartheta \sum_{i=1}^{n} s(b^i(\Delta G^s))\mathbf{L}_b^i \cdot \mathbf{N}. \tag{17}$$

Accordingly,

$$D = \frac{A - \tilde{A}}{A} = 1 - \frac{\tilde{A}}{A}. \tag{18}$$

It is the same as the original definition proposed by Kachanov (1958). For the definition with more complex mathematical forms, a further analysis associated with the damage kinetic laws can be found in Li and Woo (1993a).

6. DAMAGE BY CRACKS WITH EXPLICIT GEOMETRY AND LOCATION

When the geometry and location of one or more cracks in a solid is explicitly represented, the damage of the solid may be determined by the growth of these cracks. In this case, some mathematical formulations have been developed to provide the rigorous basis for the practical measurements of the characteristic values which represent the overall, general characteristic fracture resistance of a specific solid. A simple example is the linear elastic fracture mechanics (LEFM), from which cracks are assumed to be surrounded by a field in a homogeneous linear elastic isotropic solid. For the special case, it has been proved that there exists the so-called stress singularity at the crack tip and a complex stress field adjacent to the crack tip even under a very simple loading condition. Accordingly, a local characteristic parameter, stress intensity factor K, is introduced to describe the complex stress field near to the crack tip and then the constitutive equation of fracture kinetic is established. More practical models have been developed by assuming that the crack is surrounded by an elastic–plastic, plastic or viscoplastic material.

Relating to the characteristic size of macrocracks and microcracks to fit in with the theories developed by fracture mechanics (FM) and DM, the relation between them may be considered as a question of scale. However, if taking the fact that almost all characteristic parameters adoped by FM, such as K and J, are developed by classical theories of continuous medium, on may find that the question of scale in FM does only refer to the medium surrounded by the crack. In other words, the question of scale should not be determined by the size of cracks considered, but the medium surrounding the cracks. In fact, both FM and macro continuum damage mechanics are based on the local theory. There are two main distinctions between DM and FM:

(1) For DM, an internal variable to describe the damage of solids is introduced into the constitutive equation based on the classical mechanics of continuous media.
(2) For FM, the special geometrical boundary conditions with a sharp crack have been considered, but this is not necessary in DM.

A possible example referring to the question of scale for a solid with explicit geometry and location may be contributed by Chudnovsky and his colleagues [see Chudnovsky (1984), Chudnovsky *et al.* (1987a, b), and Chudnovsky and Wu (1990)]. A modified stress intensity factor is obtained by considering a macrocrack surrounded by a special microcrack field.

Since a macrocrack is only treated as a special geometric boundary problem, the scale parameters will be independent of the size of the crack. Accordingly, the damaged field associated with the cracked region could be represented by our proposed definition.

7. THEORETICAL AND PRACTICAL SIGNIFICANCE OF THE PROPOSED DEFINITION

The physically rigorous definition together with the geometrically consistent representation for material damage is applicable to both nonlocal and local damage theory associated with all possible scale parameters. It also provides a mathematical model to represent quantitatively the material damage caused by the metallurgical or synthetic processes. In this circumstance, the identification of damage will, of course, refer to micro material properties described by material science or solid state physics.

With respect to mechanics, the damage theory associated with the proposed definition could be developed in purely physically or physical-phenomenologically consistent manners. Based on the cardinal concepts and principles of quantum mechanics as well as the rate theory of atomic activation, the physically rigorous damage kinetic equations have been derived by Woo and Li (1993a). Referring to the multi-barrier model of the rate theory, the general damage kinetic constitutive equation is represented by the spatial discrete elementary damage kinetic equation

$$\dot{D} = (n/\Lambda_0) f(\mathbf{L}_b^i \cdot \mathbf{N})(\vec{\kappa}^{\#} - \overleftarrow{\kappa}^{\#}) \exp\left(\frac{\vec{W} + \overleftarrow{W}}{kT}\right), \tag{19}$$

or physical continuous elementary damage kinetic equation

$$\dot{D} = (n\vartheta^i/A) f(\mathbf{L}_b^i \cdot \mathbf{N})(\vec{\kappa}^{\#} - \overleftarrow{\kappa}^{\#}) \exp\left(\frac{\vec{W} + \overleftarrow{W}}{kT}\right), \tag{20}$$

where $\vec{W}$ denotes external work contributed to the forward activation and $\overleftarrow{W}$ to the backward activation. The initial bond state Λ_0 is a constant dependent on the reference state of damage and $f(\mathbf{L}_b^i \cdot \mathbf{N})$ dependent on the properties of the subsystem. The activation constant $\vec{\kappa}^{\#}$ for the forward activation is expressed as

$$\vec{\kappa}^{\#} = \vec{\kappa} \frac{kT}{h} \exp\left(-\frac{\Delta \vec{G}^{\#}}{kT}\right), \tag{21}$$

and $\overleftarrow{\kappa}^{\#}$ for the backward activation as

$$\overleftarrow{\kappa}^{\#} = \overleftarrow{\kappa} \frac{kT}{h} \exp\left(-\frac{\Delta \overleftarrow{G}^{\#}}{kT}\right), \tag{22}$$

in which κ is the transmission coefficient; h is Planck's constant; k is Boltzmann's constant; T denotes the absolute temperature; and $\Delta G^{\#}$ denotes the activated Gibbs free energy. Obviously, the identification of damage is in relation with the activated energy $\Delta G^{\#}$ which can be measured through the physical and chemical methods. This is a physically rigorous damage theory from which most damage processes in relation with complex controlling mechanisms could be described [for details, see Woo and Li (1992a, 1993a)].

The fundamental characteristics of material damage exposed by the proposed definition together with the concept of micro deformation lead to a rational synthesis for all energy dissipative mechanisms into only controlled ones, known as generalized plasticity and generalized damage [see Li and Woo (1993a)]. This enables a simple and distinct thermodynamic framework for the formulation of nonlinear response with changing material properties to be established (Li and Woo, 1993b). This is a physical and phenomenological consistent material theory, in which the dissipative potential referring to damage is derived

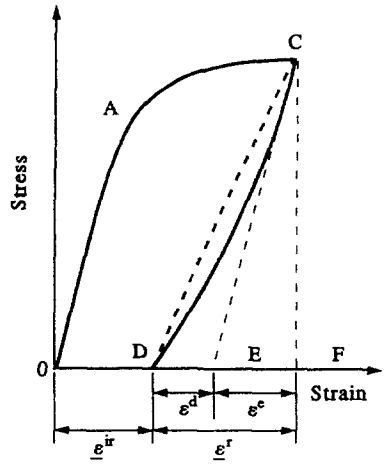

Fig. 3. Schematic illustration of the additional strain decomposition.

from the thermal activated damage kinetics established by Woo and Li (1993a). Although this proposed framework is a local damage theory referring to the zeroth longwave approximation, the phenomenological identification for damage can be carried out through the physical and chemical methods in relation to rigorous physical parameters and activated energy. The identification for damage from microcracks or microcavities is also possible by virtue of the concept of the characteristic area of the atomic bond introduced in Section 2.1 and eleborated further in Li and Woo (1993a).

We are also trying to set up the relationship between the physical properties of material damage and macro material parameters such as strength and stiffness of materials. We need to establish the special constitutive equations for nonlinear material response. The direct formulation for elasto-damage, plastic-damage and elasto-plastic-damage responses is possible by means of additional strain decomposition as shown in Fig. 3. If the unloading curve *CD* could be assumed as a straight line, damage strain tensor ε^d could be related to the elastic modulus easily. However, it has been recognized, from both the theoretical and experimental approaches, that the phenomenological identification of damage through elastic modulus alone is insufficient. In other words, although the changing microstructures referring to material damage could result in the change of elastic modulus, alteration of the elastic modulus is only the consequence of partial damage. This conclusion is supported by both experiment and theory in relation to a new physical definition for elastic response, which is based on the cardinal concept of quantum statistical mechanics.

Furthermore, the probabilistic characteristics of material damage revealed by the proposed definition of material damage lead to a physical-phenomenological-probabilistic consistent material theory [see Li and Woo (1993c)]. The evolution equations referring to the stochastic energy dissipative processes are represented by a group of independent Itô stochastic differential equations. The solutions of these equations for the stochastic internal variables defined in the probabilistic subspaces correspond to the physical diffusion processes. When the diffusion matrix H equals zero or the stochastic disturbances can be ignored, the probabilistic formulation is degenerated to the deterministic one with all the internal variables represented by the statistical mean values in which the noise-induced shift could be included. As a special case, the general stochastic dynamic model of continuum damage mechanics proposed by Woo and Li (1992b) falls into the proposed material theory. The probabilistic formulation has been confirmed by the experimental investigation carried out by Woo and Li (1993b).

8. CONCLUSIONS

For the purpose of developing a physically and geometrically consistent definition for material damage, a physically-based model is proposed. The material damage is entirely

dependent on the states of atomic bonds. The physical concepts for the definition are adhering to and extending from the elementary concepts and principles of quantum and statistical mechanics. The damage in conception has been enlarged to the phenomena not only with the reduced material stiffness and strain-softening caused by nucleation, growth, and coalescence of microcracks and microcavities, but also any changes of the microstructures in the solid. The proposed definition for material damage is applicable to most damage theories referring to different scale parameters.

The geometrical consistency for the definition could be obtained through a scheme based on a subsystem model, from which the configuration of the system of atomic bonds will be reset by the configurations of the subsystems. Through the subsystem model, the meso characteristic, such as the crystalline slip, twinning and loss of cohesion along the grain boundaries or cleavage plane as well as microcracks and voids and so on, could be described.

REFERENCES

Chaboche, J. L. (1988a). Continuum damage mechanics: Part 1. General concepts. *ASME J. Appl. Mech.* **55**, 59–64.

Chaboche, J. L. (1988b). Continuum damage mechanics: Part 2. Damage growth, crack initiation, and crack growth. *ASME J. Appl. Mech.* **55**, 65–72.

Chudnovsky, A. (1984). Crack layer theory. Case Western Reserve University, NASA Contractor Report 174634.

Chudnovsky, A., Dolgopolsky, A. and Kachanov, M. (1987a). Elastic interaction of a crack with a microcrack array—I. Formulation of the problem and general form of the solution. *Int. J. Solids Structures* **23**(1), 1–10.

Chudnovsky, A., Dolgopolsky, A. and Kachanov, M. (1987b). Elastic interaction of a crack with a microcrack array—II. Elastic solution for two crack configurations (piecewise constant and linear approximations). *Int. J. Solids Structures* **23**(1), 11–21.

Chudnovsky, A. and Wu, S. (1990). Elastic interaction of a crack with a random array of microcracks. *Int. J. Fract.* **49**, 123–140.

Edelen, D. G. B., Green, A. E. and Laws, N. (1971). Nonlocal continuum mechanics. *Arch. Rat. Mech. Anal.* **43**, 36–44.

Eringen, A. C. (1978). Nonlocal continuum mechanics and some applications. In *Nonlinear Equations in Physics and Mathematics* (Edited by A. O. Barut), Holland.

Kachanov, L. M. (1958). On the time to failure during creep. *Izv. Akad. Nauk SSSR, OTN* **8**, 26–31.

Kestin, J. and Bataille, J. (1978). Irreversible thermodynamics of continua and internal variables. In *Continuum Models of Discrete Systems* (Edited by J. W. Provan). University of Waterloo Press, Waterloo.

Kestin, J. and Rice, J. R. (1970). Paradoxes in application of thermodynamics of strained solids. In *A Critical Review of Thermodynamics* (Edited by E. B. Stuart *et al.*), pp. 275–298. Mono Book Corp., Baltimore.

Krajcinovic, D. (1984). Continuous damage mechanics. *Appl. Mech. Rev.* **37**, 1–6.

Krajcinovic, D. (1985). Continuous damage mechanics revisited: Basic concepts and definitions. *ASME J. Appl. Mech.* **52**, 829–834.

Krajcinovic, D. (1987). Micromechanical basis of phenomenological models. In *Continuum Damage Mechanics Theory and Applications, International Center for Mechanical Sciences Courses and Lecture, No. 295* (Edited by D. Krajcinovic and J. Lemaître), pp. 195–206. CISM Udine.

Krajcinovic, D. and Sumarac, D. (1987). Micromechanics of the damage processes. In *Continuum Damage Mechanics Theory and Applications, International Center for Mechanical Sciences Courses and Lecture, No. 295* (Edited by D. Krajcinovic and J. Lemaître), pp. 135–194. CISM, Udine.

Kröner, E. (1963). On the physical reality of torque stresses in continuum mechanics. *Int. J. Engng Sci.* **1**, 261–278.

Kröner, E. (Ed.) (1968). Mechanics of generalized continua. *Proc. IUTAM Symposium on the Generalized Cosserat Continuum and the Continuum Theory of Dislocations with Applications*, Freudenstadt and Stuttgart, 1967. Springer, Berlin.

Kunin, I. A. (1975). *Teoria uprugikh sred c mikrostrukturoi* (*Theory of Elastic Media with Microsructure*). Nauka, Moscow.

Kunin, I. A. (1982). *Elastic media with microstructure I. One-dimensional models.* Springer, Berlin.

Kunin, I. A. (1983). *Elastic media with microstructure II. Three-dimensional models.* Springer, Berlin.

Lemaître, J. (1987). Formulation and identification of damage kinetic constitutive equations. In *Continuum Damage Mechanics Theory and Applications, International Center for Mechanical Sciences Courses and Lecture, No. 295* (Edited by D. Krajcinovic and J. Lemaître), pp. 37–90. CISM, Udine.

Lemaître, J. (1992). *A Course on Damage Mechanics.* Springer, Berlin.

Li, D. L. and Woo, C. W. (1993a). Thermodynamic formulation for material with changing internal structures—I. Physical and phenomenological representation of damage. *Int. J. Solids Structures* (submitted).

Li, D. L. and Woo, C. W. (1993b). Thermodynamic formulation for material with changing internal structures—II. Deterministic local thermodynamic formulation. *Int. J. Solids Structures* (submitted).

Li, D. L. and Woo, C. W. (1993c). Thermodynamic formulation for material with changing internal structures—III. Probabilistic local thermodynamic formulation. *Int. J. Solids Structures* (submitted).

Rabier, P. J. (1989). Some remark on damage theory. *Int. J. Engng Sci.* **27**(1), 29–54.

Rabotnov, Yu. N. (1963). On the equations of state for creep. *Progr. Appl. Mech.* 307–315.

Rice, J. R. (1970). On the structure of stress–strain relations for time-dependent plastic deformations in metals. *ASME J. Appl. Mech.* **37**, 728–737.

Rice, J. R. (1971). Inelastic constitutive relations for solids: An integral variable theory and its application to metal plasticity. *J. Mech. Phys. Solids* **19**, 433–455.

Rice, J. R. (1975). Continuum mechanics and thermodynamics of plasticity in relation to microscale deformation mechanisms. In *Constitutive Equations in Plasticity* (Edited by A. S. Argon). The MIT Press, Cambridge.

Truesdell, C. and Toupin, R. A. (1960). The classical field theories. In *Principles of classical mechanics and field theory, Encyclopedia of Physics, Vol. III/1*. Springer, Berlin.

Woo, C. W. and Li, D. L. (1992a). On damage kinetic model with atomic activation over a system of energy barriers. In *Asia-Pacific Sym. on Advances in Engineering Plasticity and its Application*, 15–17 December, Hong Kong (Edited by W. B. Lee *et al.*). Elsevier, Amsterdam.

Woo, C. W. and Li, D. L. (1992b). A general stochastic dynamic model of continuum damage mechanics. *Int. J. Solids Structures* **29**(23), 2921–2932.

Woo, C. W. and Li, D. L. (1993a). Fundamental formulation of thermal activation damage kinetics. *Int. J. Solids Structures* (submitted).

Woo, C. W. and Li, D. L. (1993b). Statistical analysis of material damage with changing internal structure. *J. Engng Fract. Mech.* (submitted).