
Mesomechanics and Multiscale Modelling for Yield Surface

19.1 Introduction

Mechanical modelling is an abstraction, a formation of an idea or ideas that may involve the physics of solids with specific geometric configurations. Mathematical models may involve relationship between continuous functions of space and time for describing the homogeneity and/or isotropy of a material or the formation of conservation laws (Meyer, 1985; Tayler, 1986; Besseling and Liessen, 1994). The results based on these models for describing a phenomenon should agree with existing measurements within a specified accuracy and can be used with confidence to predict future observations and events.

Useful models provide valuable analogies for new situations. The challenge lies in finding a model that is simple and yields useful information, but it sufficiently diversified to give all the information required with sufficient accuracy (Meyer, 1985; Tayler, 1986; Besseling and Liessen, 1994).

Models can be built with varying degree of details at the different scale levels. A super-macro model for universe is similar a high-power telescope. A macro-model for material and structure is similar to naked eye; it takes global picture of the object at large fine details. A meso-model is similar to a low-power microscope. A micro-model is equivalent to a high-power microscope where the view of vision is narrow down to a local region giving the fine details (Meyer, 1985; Tayler, 1986). The multi-scale analysis of materials and structures on various scales are presented (Ortiz, 2008; Sadowski, 2005; Ottosen and Ristinmaa, 2005; Ma et al., 2004; 2008; Li et al., 2010; Schrefler, 2009; Zohdi and Wridggers, 2001; Ladevdz and Fish, 2003). It can be illustrated by a picture as shown in Fig. 19.1 (Li et al., 2007).

Multiscale modeling applied to meso and macro scale continuum calculations is a broad field with a long history. It encompasses hardening relations based on

dislocation density, porosity related ductile failure models, crystal plasticity, composite media and numerous other general topics dating back more than half a century. There are also a myriad of more recent activities that can be grouped under this subject heading (Becker, 2007; McDowell, 2010).

Emphasis will be placed on the research of yield criterion of element or unit cell under complex stress state in this chapter.

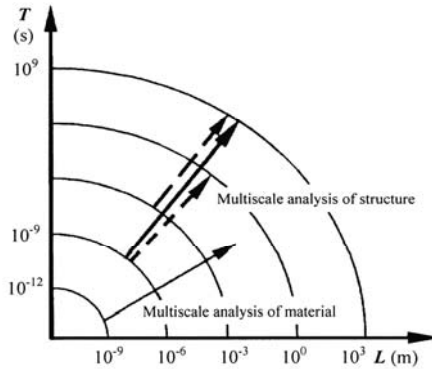


Fig. 19.1 The multiscale analysis of material and structure (Li et al., 2007)

Plastic yield criterion of metallic glass based on atomistic basis was studied by Schuh and Lund (2003). Atomic-scale study of plastic-yield criterion in nanocrystalline CU is given by Dongare et al. (2010).

The theory of the plastic distortion of a polycrystalline aggregate under combined stresses were studied by Bishop and Hill (1951), Kröner (1961) as well as Lin and Ito (1965; 1966) and others. The yield loci of polycrystalline aggregates under the combined stress (σ - τ) were studied by Lin and Ito (1965; 1966). The calculate models of Lin and Ito for polycrystalline aggregates are shown in Fig. 19.2. Three yield loci (dotted line) corresponding to the three plastic strain increment $\Delta\varepsilon=0$, $\Delta\varepsilon=0.01\times 10^{-6}$ and $\Delta\varepsilon=2\times 10^{-6}$ were given, as shown in the three dotted lines in Fig. 19.3 (Lin and Ito, 1965; 1966).

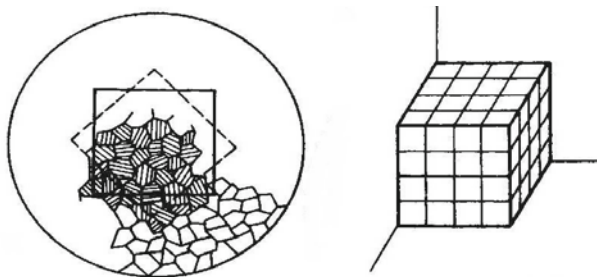


Fig. 19.2 Simulate model of polycrystalline aggregates (Lin and Ito, 1965; 1966)

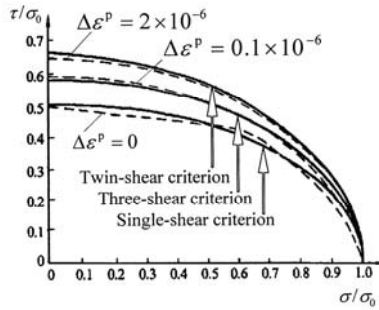


Fig. 19.3 Three yield loci of polycrystalline aggregates

The three solid lines in Fig. 19.3, top to bottom respectively correspond to the twin shear yield criterion (Yu, 1961) or the maximum deviatoric stress criterion (Haythornthwaite, 1961), three-shear yield criterion (Huber-von Mises criterion) and the single-shear yield criterion (Tresca criterion), in which the two yield loci of the Huber-von Mises criterion and the Tresca criterion were given by Lin and Ito (1965; 1966), and the third yield locus of the twin-shear yield criterion was added by Yu and Zeng in 1993 in the Collection of Papers Dedicated to Professor Tung-Hua Lin in Celebration of His 80th Birthday (Yu and Zeng, 1993).

The multi-scale analysis of materials and structures crosses wide fields of research (Becker, 2007; Ghosh et al., 1995; 1996; Ghosh et al., 2001; Tomasz Sadowski, 2005; Ottosen and Ristinmaa, 2005; Kröner, 1977; Fish and Yu, 2001; Jasiuk and Strazewski, 1994; 1998; Li et al., 2010; Liu et al., 2004, McDowell et al., 1985 to 2010; Picu, 2003; Raabe, 1998; Schrefler, 2009; Faria et al., 2010). A serial symposium and proceedings on meso-mechanics are organized and edited by Sih GC, such as the proceedings of an Int. Conf. of Role of Mechanics for Development of Science and Technology, held at Xi’an Jiaotong University, Xi’an, China, June 13-16, 2000 (Sih, 2000). A plenary lecture on material model in mesomechanics and macromechanics was presented by Yu at this Conference (Yu, 2000).

Many models have been proposed in applied mechanics. In what follows, the discussion will be confined to the strength models of materials under the complex stress state within the framework of continuum mesomechanics and macromechanics. The multi-scale analysis with emphasis on the yield surface of element (unit cell) under complex stress will be described in this chapter. The interaction yield surface of structures under combined loading is also discussed briefly. The multi-scale analysis of strength of material under various scale complex stress is illustrated as shown in Fig. 19.4.

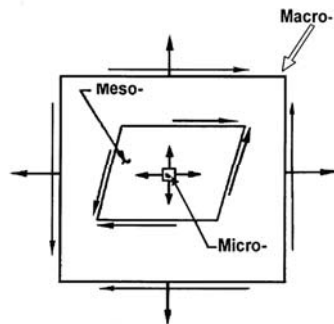


Fig. 19.4 The multi-scale analysis of strength of material under various scales of complex stress

19.2 Interaction Yield Surface of Structures

The cross-section of an element of structure, in the general case, is loaded by a combination of a normal force, bending moments at different directions, shear force, a torsion moment etc. All these quantities can be referred as the generalized force, denoted by the symbol $Q^* = Q(N_z, Q_x, Q_y, M_x, M_y, T_z)$. $N_z, Q_x, Q_y, M_x, M_y, T_z$, which are the plastic limit force of tension/compression, shear force, bending moment and torque moment, respectively. Interaction yield surface for generalized force for different structures are discussed by Hodge (1959), Save and Massonet (1972), Zyczkowski (1981), Sawczuk (1989), Stronge and Yu (1993). Detail description of interaction yield surfaces can be seen in Zyczkowski (1981).

Figure 19.5 shows the elastic-plastic state for a simply supported circular plate. The generalized yield surface, or interaction yield surface for circular plate obeying the unified yield criterion is shown in Fig. 19.6 (Liu and Jiang, 2008). Similar results can be found in structural plasticity (Yu et al., 2009) and plastic analysis of structures (Hodge, 1959; Zyczkowski, 1981, Stronge and Yu, 1993).

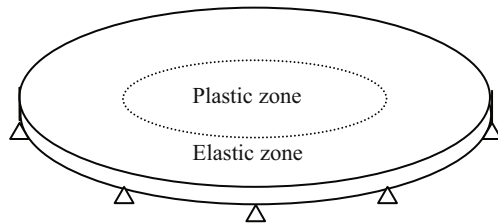


Fig. 19.5 Elastic-plastic state for a simply supported circular plate

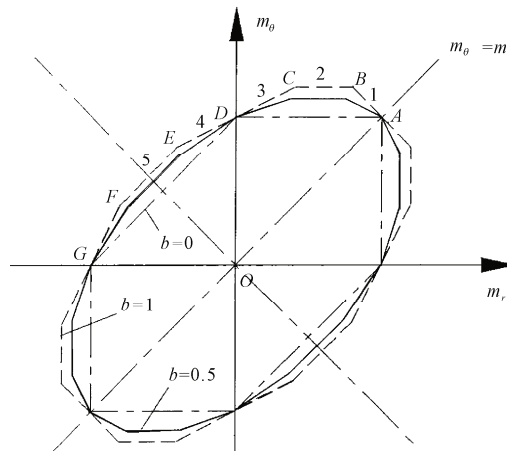


Fig. 19.6 The generalized yield surface for a circular plate obeying the unified yield criterion (Liu and Jiang, 2008)

19.3 Models in Mesomechanics and Macromechanics

A host of material models have been proposed in meso-mechanics. They include those for dislocation (Bomert et al., 1994), shear stress slip model, polycrystalline aggregate model (Lin and Ito, 1965; Dvorak and Bahei-E1-Din, 1997; Gologanu et al., 1993), equivalent inclusion (Hashin, 1962; 1983; Hashin and Shtrikman, 1964), Dugdale crack and Dugdale damage (Christeensen and Lo, 1979; Gologanu et al., 1997), continuum damage (Gurson, 1977), damage of domain of microcrack growth (Dvorak, 1999), and the differential self-consistent model etc. Continuum micro-mechanics of elastoplastic polycrystals was presented by Hill (1965).

19.3.1 RVE and HEM Model

Representative volume element (RVE) model (Hashin, 1962; 1983; Sun and Vaidya, 1996) and homogeneous equivalent medium (HEM) model are defined such that there prevails a sufficient number of volumes or subvolumes, subjected to macroscopically uniform stress, strain, or temperature change. The bulk properties are not dependent on its size (de Buhan and de Pelice, 1997). RVE model and HEM model have been used widely in mesomechanics.

19.3.2 Equivalent Inclusion Model

The elastic field for an ellipsoidal inclusion has been determined in Hashin (1962). The important result is that the strain field in the inclusion is uniform.

19.3.3 CSA and CCA Models

A direct and simple way to represent the matrix connectedness of a composite material was proposed. The composite spheres assemblage (CSA) model applies to an isotropic particulate while the composite cylinders assemblage (CCA) model introduced later has been used for fiber-reinforced transversely isotropic materials. The latter pertains to unbounded set of contiguous similar composite spheres of all sizes, including those that tends to zero such that the voids between the sphere could be filled.

19.3.4 Gurson Homogenized Model

The Gurson homogenized model (Gurson, 1977) for porous ductile metals is based on an approximate limit-analysis for hollow spheres made of rigid ideal-plastic material using the von Mises yield criterion. Some Gurson models consider the influence of void shape. The effect of strong gradients of macroscopic fields were proposed.

19.3.5 Periodic Distribution Model

Figure 19.12 shows some isotropic distributed patterns of periodic distribution model (PDM) (Christeensen and Lo, 1979).

19.3.6 PHA Model and 3-Fold Axissymmetrical Model

The periodic hexagonal array (PHA) model deals with a microstructure that consists of hexagonal and dodecahedral cylindrical fibers (Gologanu et al., 1993). A 3-fold axis of rotational symmetry model has been proposed (Dvorak and Bahei-E1-Din, 1997).

19.3.7 A Unit Cell of Masonry

A continuum model for assessing the ultimate failure of masonry as a homogenized material can be found in the literature. The unit cell is a rhombic model. Several other models have been used in the analyses of reinforced concrete and reinforced plastic.

19.3.8 Topological Disorder Models

Disorder models dispersion patterns of fibres were proposed (Pyrz and Bochenek, 1998).

19.3.9 Random Field Models of Heterogeneous Materials

The random field models of heterogeneous materials were presented by Ostoja-Strazewski (1993; 1994; 1998).

The idea of a unit cell and other models were used. Several models of composite and heterogeneous materials were presented (Hashin, 1962; I Gurson, 1977; Christeensen and Lo, 1979; Ostoja-Strazewski, 1993; 1994; 1998; Dvorak and Bahei-E1-Din, 1997; Pyrz and Bochenek, 1998; Dvorak, 1999), which are shown in Fig. 19.7.

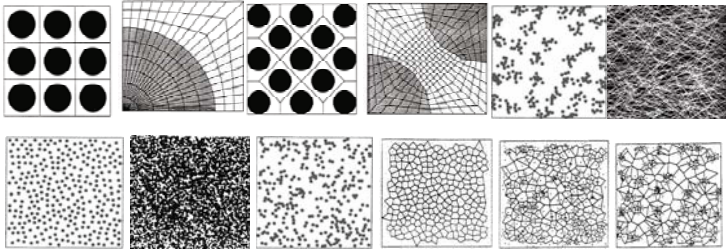


Fig. 19.7 Several models of composite and heterogeneous materials

19.4 Failure Surface for Cellular Materials under Multiaxial Loads and Damage Surfaces of a Spheroidized Graphite Cast Iron

In many applications, foams, including rigid polymer foam, lightweight cellular concrete, metallic foams and ceramic foam are subjected to multiaxial stresses. Systematic investigations regarding the multiaxial failure of foams were done at MIT (Massachusetts Institute of Technology), Cambridge University and Harvard University. Failure surfaces for cellular materials under multiaxial loads are presented by by Gibson and Ashby (1987; 1997), Gibson et al. (1989), Triantafillou and Zhang (1989), Triantafillou and Gibson (1990), Theocaris (1991), Ashby et al. (2000), Deshpande and Fleck (2000), Gibson (2000), Gioux et al. (2000), Sridhar and Fleck (2000). A yield surface is developed using an analysis of an idealised foam. It may be referred to as the GAZT (Gibson et al., 1989) yield surface. The failure criterion for tensile rupture of foams is written as follows:

$$F(I_1, J_2) = \pm\sqrt{J_2} - 0.2aI_1 = \sigma_{cr} \quad (19.1)$$

This equation is similar to the Drucker–Prager criterion for soils. The limit surfaces in stress space consist of two intersecting surfaces of conical shape associated with the tensile and compressive limit (Triantafillou and Gibson, 1990).

The yield surfaces of aluminum alloy foams for a range of axisymmetric compressive stress states have been investigated by Deshpande and Fleck (2000). The yield surfaces of compacted composite powders under triaxial testing were measured and studied by Sridhar and Fleck (2000). A design guide for metal foams was given by Ashby et al. (2000). A review for mechanical behavior of metallic foams was given by Gibson (2000).

Aluminum foams are currently being considered for use in lightweight structural sandwich panels and in energy-absorption devices. In both applications, they may be subjected to multiaxial loads. Designers require a criterion to evaluate the combination of multiaxial loads that cause failure. The Drucker-Prager criterion and a yield surface for compaction of powders are used. Both phenomenological yield surfaces give a description of the multiaxial failure of the aluminum foams tested by Gioux et al. (2000).

Multi-axial yield behaviour of polymer foams is found to be described adequately by the inner envelope of a quadratic function of mean stress and octahedral-shear stress and a maximum compressive principal stress criterion (Deshpande and Fleck, 2000).

The global extremal yield surfaces of a unit cell are constructed with the numerical experiments by Schrefler (2009).

The Huber-von Mises type functions are always used in damage mechanics (Kachanov, 1986; Lou, 1991; Lemaitre, 1992; Yu and Feng, 1997; Voyiadjis et al., 1998). A theoretical and experimental study of damage surfaces for spheroidized graphite cast iron was presented by Hayakawa and Murakami (1998) and Murakami et al. (1998). Damage evolution and fundamental aspects of damage surface of a spheroidized graphite cast iron were observed. The existence and the development of the damage surface, together with the condition of loading, unloading and neutral loading, are elucidated. The initial, subsequent and final damage surfaces were obtained by Hayakawa and Murakami (1998), as shown in Fig. 19.8.

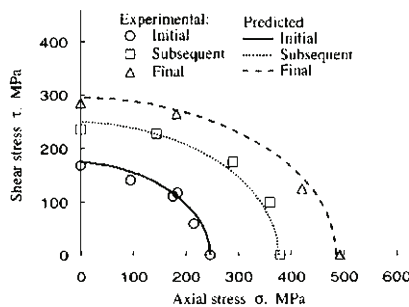


Fig. 19.8 Damage surfaces under combined stress space (Hayakawa and Murakami, 1998)

The damage surfaces can be described by a first quadrant of an ellipse in the space of axial tensile and shear stress. The ellipse of the initial damage surface has the aspect ratio of $\sigma/\tau=1.46$, the ellipse of the subsequent damage surface is $\sigma/\tau=1.62$, which are in contrast to the ellipse ($\sigma/\tau=1.733$) of the initial yield surface of von Mises type yield criterion. A theoretical damage surface under

combined stress was proposed by Murakami et al. (1998), it is closed to the experimental results as shown in Fig. 19.8.

It is interesting that the ellipse of the initial damage surface has the aspect ratio of $\sigma/\tau=1.46$, which is closed well to the twin-shear yield criterion with the ratio of $\sigma/\tau=1.5$. A twin-shear damage surface, a generalized twin-shear damage surface or the unified typed damage surface may be available. The generalized twin-shear strength criterion (Yu, 1985) and the unified strength theory (Yu, 1991) can be matched to the pressure sensitively materials.

19.5 Mesomechanics Analysis of Composite Using UST

The strength prediction for composite materials is very important in engineering. The homogenization method by using a unit cell is an effective method to evaluate the elastic stiffness property for the composite materials by many researchers. Micromechanical analysis of composite by the method of unit cell was summarized and reviewed by Aboudi (1989), Pindera and Aboudi (1989), Ju and Tseng (1996), Zhu et al. (1998). The analysis leads to the prediction of the overall behavior of various types of composites from the known material properties of fiber and matrix. The capability of the theory in providing the response of elastic, thermoelastic, viscoelastic, and viscoplastic composites, as well as their initial yield surfaces, strength envelopes, and fatigue failure curves, is demonstrated by Aboudi (1989).

The evaluations of strength of composites under the biaxial stresses by using the unified yield criteria were given by Li YM and Ishii (1998a; 1998b). A series of biaxial loads were applied to the laminate sample of boron fiber unidirectional reinforced aluminum in material principal directions, and through a meso-unit-cell to get the corresponding macroscopic elasto-plastic behavior. The unified yield criterion was used as an elasto-plastic flow potential function to evaluate strength of composite. This approach ensures the uniformity of the stress field and has no any so called slip generally in the grips during the experiment. It means that one can get a preliminary understanding of the macroscopic nonlinear elasto-plastic properties easily by numerical analysis. The corresponding FEM analysis system were developed by Quint Co. in Japan (1993; 1994).

For the flow potential function at the mesoscopic level, the unified yield criterion was used (Li and Ishii, 1998). The coefficient b in the unified yield criterion could be determined by pure shear test. Since the pure shear test is usually difficult to be carried out, the b can be taken in a range of $0 \leq b \leq 1$ for various materials. Equation (10.2) should be turned to be the Tresca yield criterion when $\alpha=1$ and $b=0$, or the Twin Shear Stress (TSS) criterion (Yu, 1961) when $\alpha=1$ and $b=1$, or it is closes to the Huber von Mises yield criterion with linearity when $\alpha=1$ and $b=0.5$. It is easy to find that the coefficient b is obviously a parameter reflecting the strength property on π -plane when stress state is close to the pure shear stress state. In fact, include all possible existing criteria which

satisfy the convex postulate on π -plane by $0 \leq b \leq 1$. So, one can select a different value of b for using different yield function by installing the unified yield criterion only into FE-code.

The unified yield criterion was used in meso-unit-cell for getting macroscopic elasto-plastic responses. This model can be considered as an experimental sample of the unidirectional reinforced laminate, and the biaxial uniform loading is applied to the two directions X_1 and X_2 as shown in Fig. 19.9.

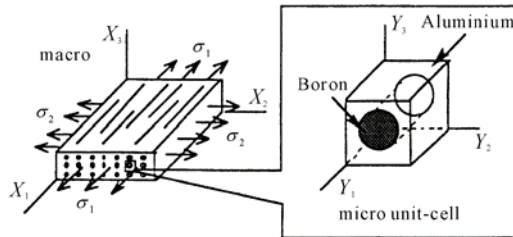


Fig. 19.9 The sample model: macro and meso

The meso-scopic properties for fiber and matrix are:

Boron: $E_f = 413.7$ GPa, $\nu_f = 0.21$, $\sigma_f^0 = 3200$ MPa;

Aluminum: $E_m = 68.9$ GPa, $\nu_m = 0.33$, $\sigma_m^0 = 262$ MPa.

Here, it is assumed that the boron fiber and aluminum matrix are of ideal elasto-plastic properties.

Figure 19.10(a) is the stress-strain properties for the tension loading in fiber direction only, and it is found that there is almost no difference among the macroscopic stress-strain curves with three yield criteria. For the tension loading in transverse direction only, however, the nonlinear stress-strain curves appear very different as shown in Fig. 19.10(b).

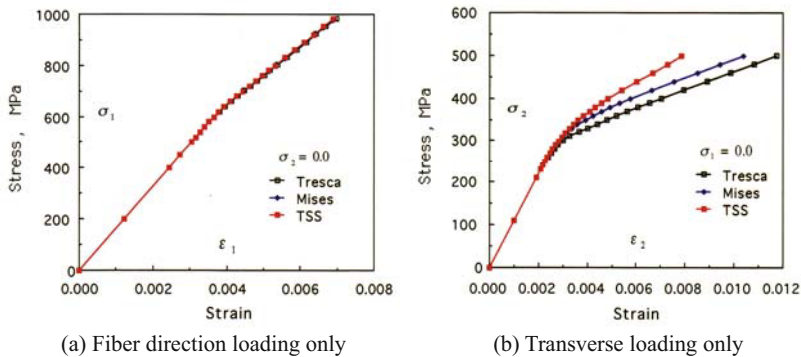


Fig. 19.10 Stress-strain curves for composite (Li and Ishii)

Obviously, the difference of nonlinear stress-strain properties is depended on the load condition by using various yield criteria at meso-scopic level. The plastic zones with different yield criteria are shown in Fig. 19.11. Figure 19.11 shows that the twin-shear yield criterion (Yu, 1961) gives a smaller plastic zone, and the single-shear yield criterion (Tresca, 1864) gives a bigger plastic zone in the unit-cell under same load.

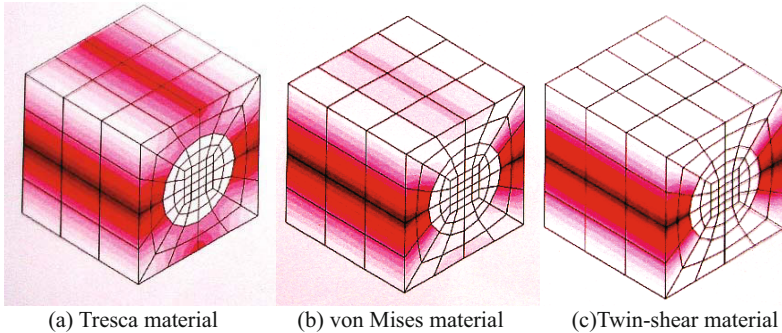


Fig. 19.11 Plastic zones in meso-unit-cell under same load (Li and Ishii)

The conclusion obtained by Li and Ishii is that the installation of the unified yield criterion makes it easy to use various yield criteria to evaluate the strength property of composite.

The unified yield criterion and the approach Li and Ishii used may be extended for more complex meso-construction composite materials, such waved fiber, honeycomb, of which the strength relation evaluation between macro and micro is not very clear until now.

The unified strength theory give us with a effect and powerful theoretical basic to study the effect of failure criterion on the evaluation of elasto-plastic behaviour of composite and other materials at macro and meso levels. Multiscale modelling of damage and fracture processes in composite materials was summarized by Sadowski (2005).

19.6 Multiscale Analysis of Yield Criterion of Metallic Glass Based on Atomistic Basis (Schuh and Lund, 2003)

Plastic yield criterion of metallic glass based on atomistic basis was studied by Schuh and Lund in 2003. The simulation model on atomistic basis is shown in Fig. 19.12 (Schuh and Lund 2003; Lund and Schuh, 2005).

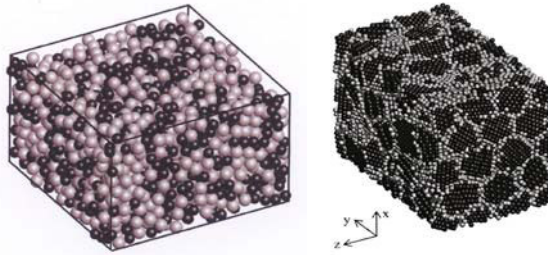


Fig. 19.12 Simulation model on atomistic basis (Schuh and Lund, 2003)

The two simulation results of metallic glass under plane stress on atomic basis given by Schuh and Lund are shown in Fig. 19.13 and Fig. 19.14. It indicated that metallic glass is tension-compression asymmetry; the Huber von Mises criterion and the Tresca criterion cannot be adapted for metallic glass. The comparison of the simulation results of yield locus with the Mohr-Coulomb yield locus (solid line) is shown in Fig. 19.14.

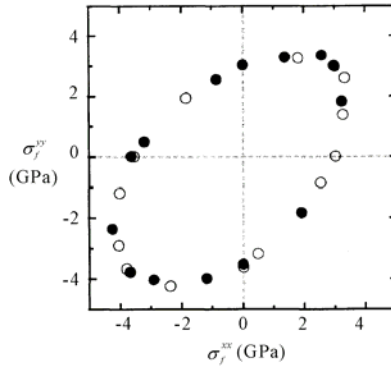


Fig. 19.13 Simulation results (Schuh and Lund, 2003)

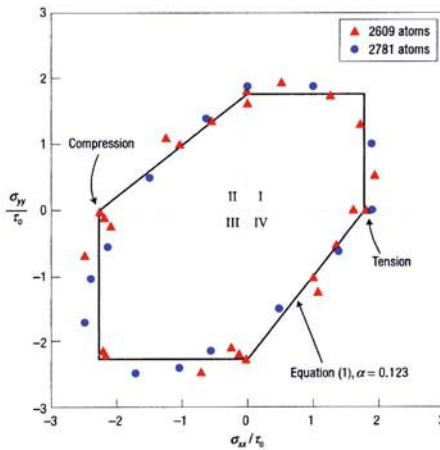


Fig. 19.14 Simulation results (Schuh and Lund, 2003)

19.7 Multiscale Analysis of Yield Criterion of Molybdenum and Tungsten Based on Atomistic Basis (Groger et al., 2008)

Multiscale modeling of plastic deformation of molybdenum and tungsten is studied by Groger et al. (2008). Yield surface for single crystals based on atomistic studies is obtained by Groger et al. as shown in Fig. 19.15.

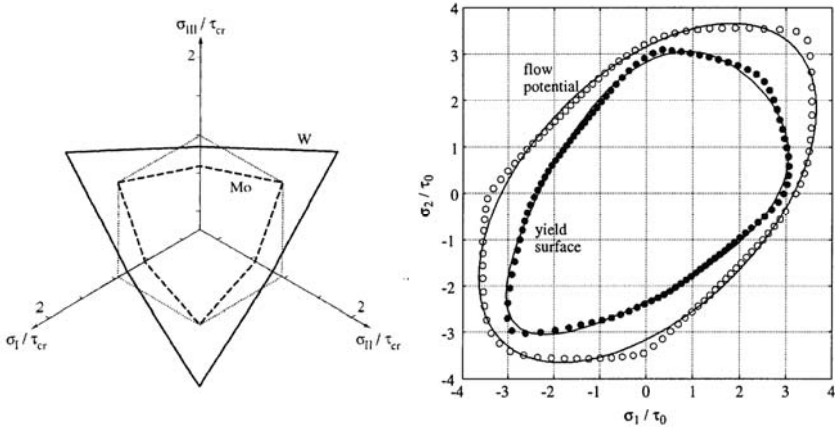


Fig. 19.15 Yield and flow surfaces predicted from a Taylor model for bcc Mo (Groger et al., 2008)

Simple isotropic functions that accurately describe computed yield and flow surfaces for random bcc poly-crystals obtained from calculations, such as those shown in Fig. 19.15, are given by Groger (2008). They constructed the analytical yield criteria as

$$F = \sqrt{3}[(J_2)^{3/2} + bJ_3]^{1/3}; \quad G = \sqrt{3J_2} \tag{19.2}$$

where $J_2 = s_{kl}s_{kl} / 2$ and $J_3 = s_{ij}s_{jk}s_{ki} / 3$ are the second and third invariants of the deviatoric stress tensor.

19.8 Phase Transformation Yield Criterion of Shape-Memory Alloys

Mechanical behavior and yield surface of shape memory alloy (SMA) under multiaxial stress has been studied widely. It has been found that the “yield” (transformation start stress in stress induced phase transformation) surface does neither really match the Huber-von Mises yield criterion nor the Tresca yield

criterion. The possibility of using such a “yield” surface to predict the behavior of a SMA under other stress conditions. “Yield” surfaces of shape memory alloys and their applications were studied by Huang (1999), Lim and McDowell (1999), Gall et al. (1998), Novák and Šittner (2004) The “yield” surfaces of four polycrystalline SMAs (NiTi, NiAl, CuZnGa, and CuAlNi) are investigated by Lexcellent et al. (2002; 2004; 2007; 2010). Phenomenological simulation of yield surfaces of NiTi polycrystal for different temperatures was presented by Lexcellent et al. (2002). A generalized macroscopic J_2 - J_3 criterion to describe the transformation onset is proposed and identified (Bouvet et al., 2002). Determination and transport of phase transformation yield surfaces for shape memory alloys are also given by Gibeau, Laydi and Lexcellent (2010). Yield surface of Cu-Al-Be polycrystalline was presented by Lexcellent et al. (2004).

Experimental yield surface of phase transformation initiation for bicompression and tension (compression)–internal pressure tests for CuAlBe polycrystalline was obtained by Lexcellent et al. (2002; 2007; 2010). A general formula to describe these “yield” surfaces is found by Lexcellent et al. The parameters in this formula can be calculated by using the “yield” stresses of tension and compression of a particular SMA. The analytical results agree well with reported experimental data of NiTi.

The simulation and experimental yield surfaces of phase transformation for shape memory ally (Lexcellent, 2010), as shown in Fig. 19.16.

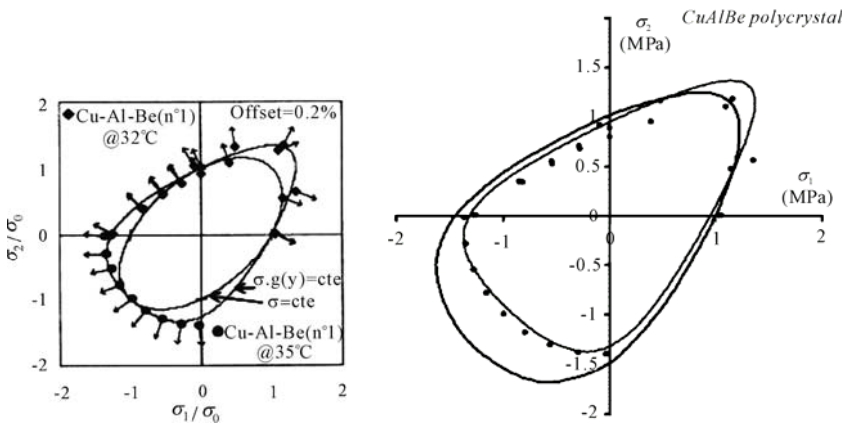


Fig. 19.16 Simulation and experimental yield surface of phase transformation for CuAlBe shape memory alloy (Lexcellent, 2010)

A new yield surface is presented by Kolupaev and Altenbach (2010), which is illustrated by red line in Fig. 19.17. It is interesting that the Kolupaev-Altenbach yield surface is similar to the simulation and experimental yield surfaces of shape memory alloy, as shown in Fig. 19.16 (Lexcellent, 2010).

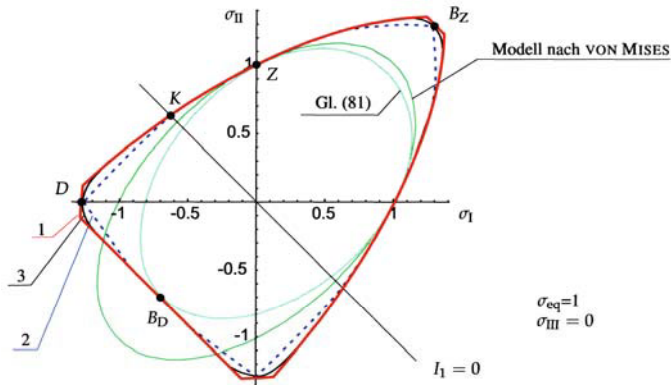


Fig. 19.17 New yield surface (Kolupaev-Altenbach, 2010)

The transformation yield surface of shape-memory alloys was also studied by Bhattacharya and Schlömerkemper (2004).

19.9 Atomic-Scale Study of Yield Criterion in Nanocrystalline CU

Atomic-scale study of plastic-yield criterion in nanocrystalline CU is given by Dongare et al. (2010). Initial configuration of nanocrystalline Cu with an average grain size of 6nm. System consists of approximately 1.2 million atoms arranged in 122 grains, as shown in Fig. 19.18. Molecular dynamics (MD) simulations for yield surface are presented. Plot of the calculated yield stress and flow (peak) stress in tension and compression at strain rates $1 \times 10^9 \text{ s}^{-1}$ to $8 \times 10^9 \text{ s}^{-1}$, respectively is given in Fig. 19.19. It is seen that yield stress and limit stress values are greater in compression and the difference increases with increasing strain rates. So, the single parameter yield criterion cannot be adopted for nanocrystalline CU.

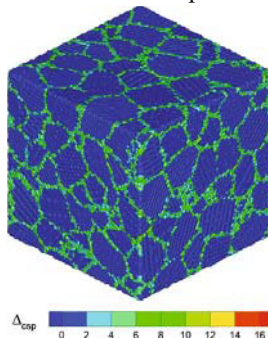


Fig. 19.18 Initial configuration of nanocrystalline Cu with an average grain size of 6 nm

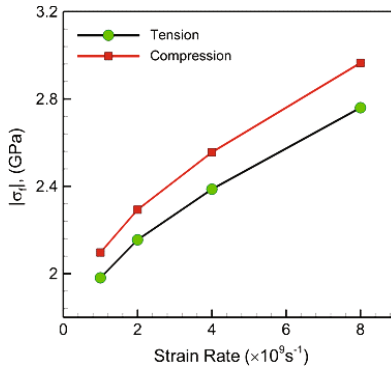


Fig. 9.19 Plot of the calculated yield stress and limit (peak) stress in tension and compression

In the work of Dongare et al. (2010), the biaxial yield surface is calculated by plotting the yield/limit stresses during loading of the nanocrystalline metal by equal/unequal amounts in the X and Y directions and keeping the stress in the Z direction constant ($\sigma_x = \sigma_1$, $\sigma_y = \sigma_2$, and $\sigma_3 = \sigma_z = 0$). The calculated yield stresses and limit stresses under combined biaxial loading conditions (X - Y) give a locus of points that can be described with a traditional ellipse. However, the center of the ellipse deviated from the center of coordinate (solid lines) a small value, as shown in Fig. 19.20. Dashed lines indicate the shifted center of the ellipse.

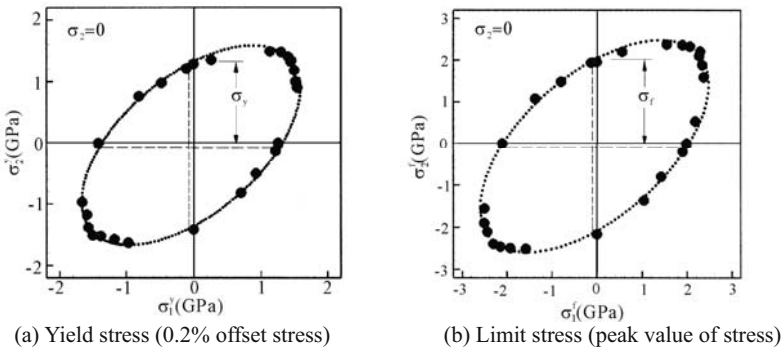


Fig. 19.20 Yield loci for biaxial loading in the X and Y directions and zero stress in the Z direction

The deviation of shifted center of the ellipse is due to the SD (Strength Difference) effect of material, or the tension-compression asymmetry in yield stress and limit stress. It is need to find other theory and method to match these results. A two-parameters yield criterion (or limit criterion), which the SD effect is taken into account, is necessary. The strength ratio of material in tension and in compression $\alpha = \sigma_t / \sigma_c$ is introduced that allows for the incorporation of the tension compression asymmetry. The strength ratio of material in tension and in

compression is $\alpha = \sigma_t / \sigma_c = 0.88$ to $\alpha = \sigma_t / \sigma_c = 0.9$ in this case. The traditional von Mises yield criterion and Tresca yield criterion cannot be fitted to the results.

It is interesting that the results are situated between two convex bounds, as shown in Fig. 19.21. The SD effect is taken into account in these two convex bounds. The inner bound (dotted line) is the Mohr-Coulomb theory.

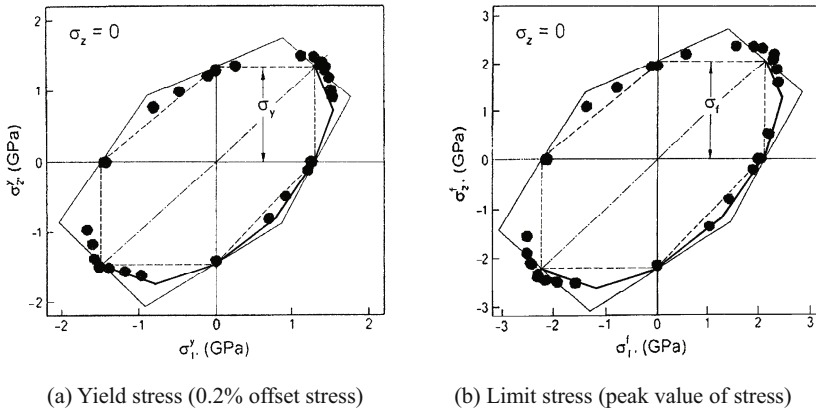


Fig. 19.21 The results situated between two convex bounds

19.10 A General Yield Criteria for Unit Cell in Multiscale Plasticity

Consider a unit cell on the mesoscale with the length of all edges equal to l_e , as shown in Fig. 19.22. Within this unit cell, the cell is sufficiently small, higher order displacement gradients can be ignored and the strain field varies linearly as the Hooke law. It is assumed that the essential structure of conventional plasticity is preserved on the micro-scale. The Huber-von Mises criterion was always used as the micro-scale effective stress and strain analysis.

In general, the yield behaviour of unit cell in meso-scale and micro-scale is always strength asymmetric in tension and in compression. So, a two parameter yield criterion is need.

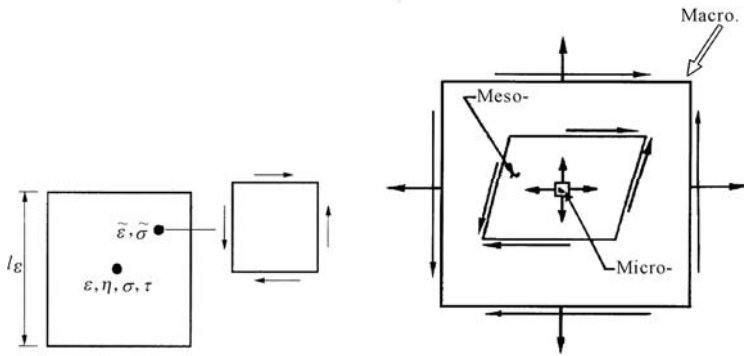


Fig. 19.22 Macro-meso-micro analysis of element (or unit cell) under complex stress

The material models are widely used in mesomechanics and macromechanics. It is hopeful that a simple model could be found to give useful information. It should also be sufficiently general and yield accurate results. Moreover, the formulation should contain the least number of state variables.

It is assumed that:

- 1) The strength of unit cell at different direction is identical, but the strength is different in tension and in compression. The cell is a SD material. The SD material is also referred as strength asymmetrical in tension and in compression.
- 2) The strength of unit cell is different at different scales. Denoted the strength as Σ'_v , tensile strength of unit cell, Σ^c_v , compressive strength of unit cell.
- 3) The principal stresses acted on the each sides is denoted as Σ_1, Σ_2 and Σ_3 .

So, the single parameter criteria, such as the Tresca criterion, the Huber-von Mises criterion and the twin-shear single parameter criterion (Yu, 1961) or the maximum deviatoric stress criterion (Schmidt, 1932; Ishlinsky, 1940; Hill, 1950; Haythornthwaite, 1961, see: Chapter 3) cannot be adopted.

According to the UST, a simple general yield criterion for unit cell may be proposed as follows:

$$F = \Sigma_1 - \frac{\alpha}{1+b}(b\Sigma_2 + \Sigma_3) = \Sigma_t, \text{ when } \Sigma_2 \leq \frac{\Sigma_1 + \alpha\Sigma_3}{1+\alpha}, \tag{19.3a}$$

$$F' = \frac{1}{1+b}(\Sigma_1 + b\Sigma_2) - \alpha\Sigma_3 = \Sigma_c, \text{ when } \Sigma_2 \geq \frac{\Sigma_1 + \alpha\Sigma_3}{1+\alpha} \tag{19.3b}$$

where $\alpha = \Sigma'_t / \Sigma^c$ is strength ratio of unit cell in tension and in compression. b is a parameter for the choice of yield criterion.

The yield loci of this criterion in plane stress state are illustrated in Fig. 19.23 for two different ratio of $\alpha = \Sigma'_t / \Sigma^c$.

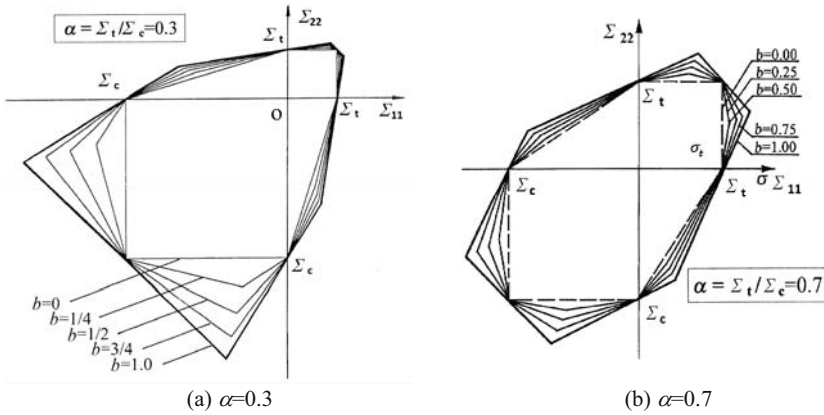


Fig. 19.23 Strength difference in tension and in compression

This general yield criterion for unit cell can be also extended to the non-convex yield loci when the parameter $b < 0$ or $b > 1$. The convex yield loci and non-convex yield loci of the unified yield loci of unit cell for $\alpha=0.5$ material are shown in Fig. 19.24. Many problems regarding the non-convex yield surface remain open. A Plenary Lecture on “Nonconvex Plasticity and Microstructure” was presented by Ortiz at 22nd International Congress of Theoretical and Applied Mechanics, Adelaide, Australia, August 27, 2008.

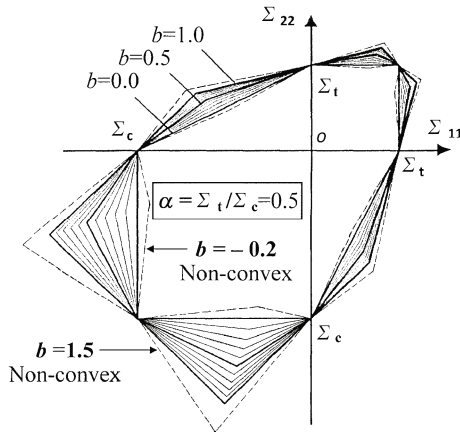


Fig. 19.24 Convex yield loci and non-convex yield loci

This general yield criterion for unit cell is a very simple criterion. However, it is better to match many new results. The calculative results of metallic glass at atomic base have been obtained by Schuh et al. (2003; 2005), as shown in Figs. 19.13 and 19.14. They are shown again with the comparison to yield criterion in Fig. 19.25 and Fig. 19.26. The yield surfaces of simulation results for metallic glass are convex and strength asymmetric in tension and in compression,

which are situated between the two bounds as shown in Fig. 19.25. The comparisons of the UST $b=0$ (inner bound), $b=0.5$ (median) and $b=1$ (upper bound) with simulation result of Schuh et al. are given.

Obviously, the results show the strength asymmetric in metallic glass (Schuh and Lund, 2003). The Tresca criterion and Huber-von Mises criterion cannot be adopted. The Mohr-Coulomb criterion may be used for match the results. It is noted that the general yield criterion for unit cell with $b=0.5$ is also adapted for this result, as shown in Figs. 19.25 and 19.26.

Atomic-scale study of plastic-yield criterion in nanocrystalline CU is given by Dongare, et al. (2010), as stated in section 19.9. The results indicate that:

1) The strength of nanocrystalline CU is tension-compression asymmetry. It has been indicated in Fig. 19.20. The strength ratio of material in tension and in compression is $\alpha=\sigma_t/\sigma_c=0.88$ to $\alpha=\sigma_t/\sigma_c=0.9$. So a two-parameter yield criterion is needed.

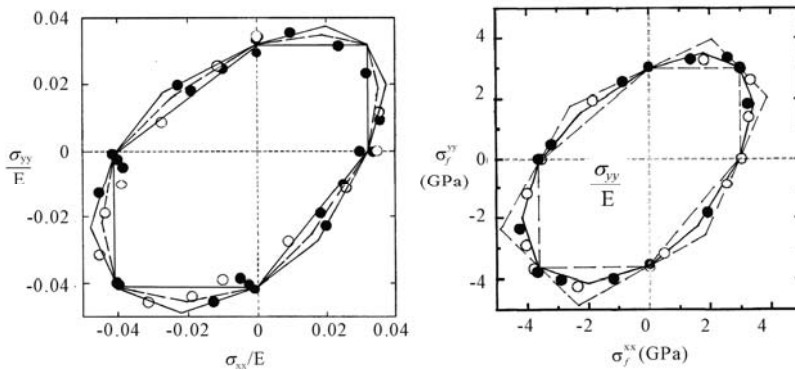
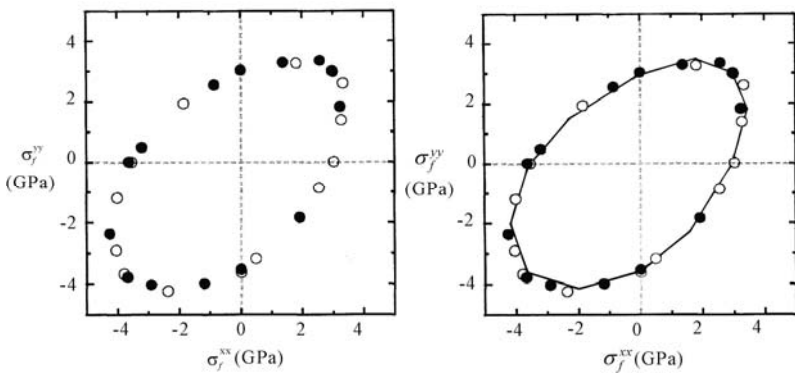


Fig. 19.25 Comparison of the UST $b=0, b=0.5$ and $b=1$ with simulation result of Schuh et al.



(a) Simulation results for metallic glass (b) Match of simulation results with $b=1/2$

Fig. 19.26 Comparison of the UST $b=0.5$ with simulation result of Schuh et al.

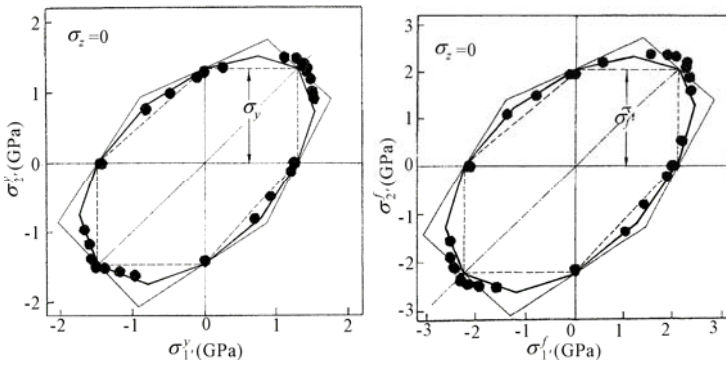


Fig. 19.27 The comparison of the calculated yield loci and the general yield criterion for unit cell with parameter $b=1/2$

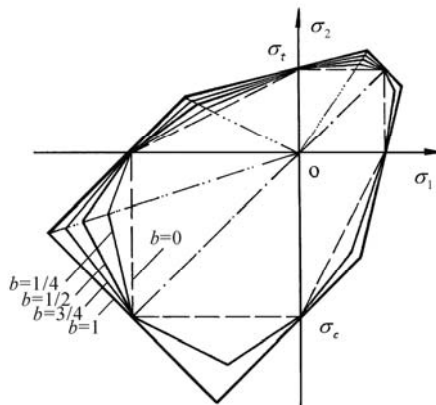
2) The yield loci (yield locus and limit locus) obtained from MD simulations are situated between two convex bounds, as shown in Fig. 19.21.

3) The calculated biaxial yield loci for the yield stress and limit stress can be fit to the general yield criterion for unit cell, described in equations 19.3a and 19.3b. A series of yield loci is shown in Figs. 19.23 and 19.24.

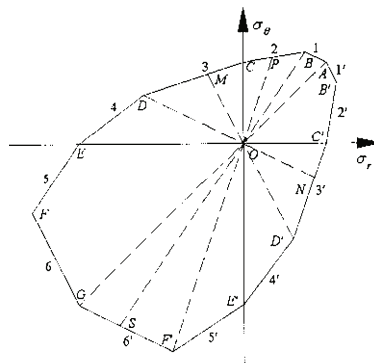
4) Significant work is needed to evaluate the parameter b to plasticity under multiaxial loading conditions and, in turn, the yield criterion to predict the macroscopic behavior of these metals at different loading conditions.

5) The comparison of the calculated biaxial yield surface for the yield and limit stresses and the general yield criterion for unit cell with parameter $b=1/2$ are shown in Fig. 19.27.

The shape of yield loci of the unified strength theory will be changed if the strength ratio of material in tension and in compression $\alpha=\sigma_t/\sigma_c$ is decreased. Fig. 19.28 shows the yield loci of the unified strength theory with five typed cases ($b=0, b=1/4, b=1/2, b=3/4, b=1$) and three typed cases ($b=0, b=1/2, b=1$) when the strength ratio of material in tension and in compression $\alpha=\sigma_t/\sigma_c=1/2$.



(a) UST with five and three typed cases



(b) UST with $b=1/2$

Fig. 19.28 Yield loci of the UST in plane stress state (for $\alpha=\sigma_t/\sigma_c=1/2$ material)

19.11 Virtual Material Testing Based on Crystal Plasticity Finite Element Simulations

The CPFE (Crystal Plasticity Finite Element) method is studied systematically by Raabe et al. (Raabe, 1998; Kraska et al., 2009; Roters et al., 2010). The effects of microstructure and texture and their evolution during deformation are taken into account. The example in this section presents an application of the CPFE method for the concept of virtual material testing using a representative volume element (RVE) approach (Kraska et al., 2009). By using such numerical test protocols it becomes possible to determine the actual shape of the yield locus, and to use this information to calibrate empirical constitutive models used. Along with standard uniaxial tensile tests, other strain paths are numerically monitored, such as biaxial

tensile, compressive or shear tests. The use of the CPFE method for virtual testing of yield locus is demonstrated by Roters et al. for a low-carbon steel grade.

19.12 Meso-Mechanical Analysis of Failure Criterion for Concrete

The computational modelling of failure criteria for concrete materials was studied by Buyukozturk et al. (1970), and Liu et al. (1972). The unit cell of concrete combined by circular aggregate and mortar was used. Needleman (1994) gave a summary relating the computational modelling of materials failure.

The model of concrete composited by circular aggregate and mortar is shown in Fig. 19.29. The failure criterion for concrete was obtained by Liu et al. (1972) as shown in Fig. 19.30, in which the dotted lines is the analysis result, and the solid point is the experimental result.

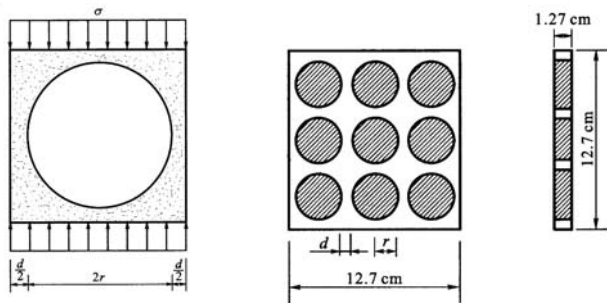


Fig. 19.29 Analysis model of concrete composited by circular aggregate and mortar

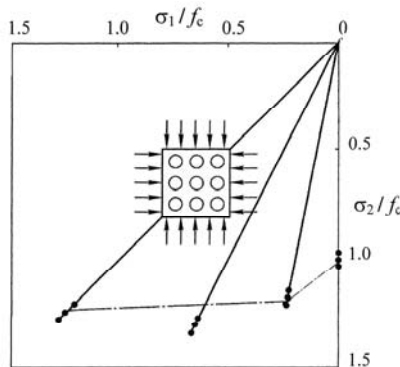


Fig. 19.30 Simulated limit locus for concrete under biaxial compression (Liu et al., 1972)

The computational simulation of failure criterion for concrete was done by Yu and Zeng (1993) and Zeng and Wei (1998). The concrete was regarded as a

composite material composed of big aggregates (1), small aggregates (2), water bubble (3), air bubble (4), and mortar (5) as shown in Figs. 19.31 (a)~19.31(c). The Unified Elasto-Plastic Program and the twin-shear strength theory were used under plane stress condition and plane strain condition.

Various stress combinations were calculated. Different model and different stress state $\sigma_1, \sigma_2, \sigma_3=0$ ($\varepsilon_3 \neq 0$) gave different limit value. Twenty-two stress combinations were calculated as shown in Fig. 10.32. The failure locus of concrete with big aggregate is smallest, and anisotropic. The failure loci obtained according to three meso-models are shown by the solid curve, the dotted curve and the broken curve, respectively. The horizontal compressive strength of model with big aggregate is larger than that of vertical. The failure locus of concrete becomes larger and isotropic when the size of aggregates decreased.

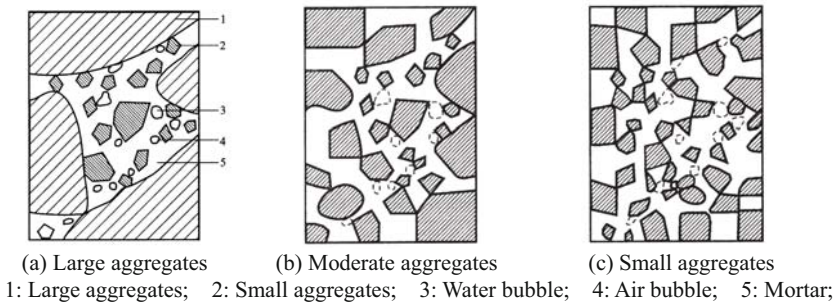


Fig. 19.31 Three meso-concrete models with different aggregate gradation

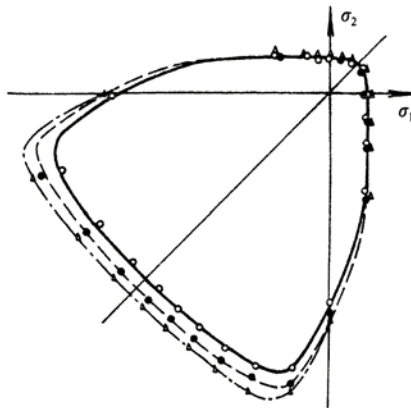


Fig. 19.32 Failure loci of three meso-concrete models under plastic stress conditions

Figure 19.33 shows the computational failure loci of the meso-model under the plane strain condition $\sigma_1, \sigma_2, \varepsilon_3=0$ ($\sigma_3 \neq 0$) by using of the Mohr-Coulomb strength theory and the twin-shear strength theory. The outer failure locus (line 2) is obtained using the twin-shear strength theory, and the inner failure locus (line 1) is obtained using the Mohr-Coulomb strength theory. The solid points are the

experimental results. The biaxial compressive strength of concrete at the compressive stress zone under the plane strain condition is larger than that of the plane stress condition, which agrees with the experimental results.

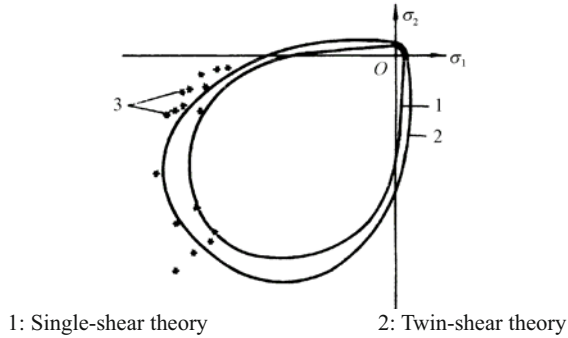


Fig. 19.33 Failure loci of meso-concrete models under plastic strain condition

Recently, a meso-mechanical analysis of concrete specimens under biaxial loading was presented by Caballero et al. (2007). Finite element mesh for concrete and rigid platens and numerical results under plane stress are shown in Fig. 19.34. Seventeen simulation results (above the diagonal $\sigma_1 = \sigma_2$) under different loading paths with different proportions of σ_1 and σ_2 are obtained as shown in Fig. 19.34. The failure locus is obtained by connecting these 17 points and using the symmetric condition about the diagonal $\sigma_1 = \sigma_2$.

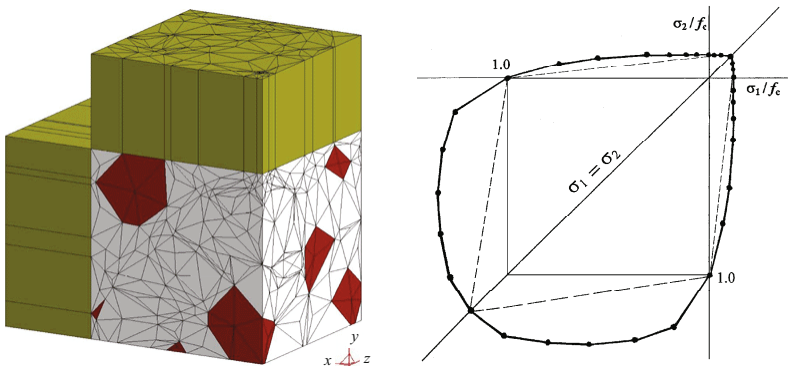


Fig. 19.34 FE mesh for concrete and rigid platens and numerical failure locus for concrete under plane stress (Caballero et al., 2007)

The results show that the tensile strength and compressive strength of concrete is different ($f_t \neq f_c$). It means that the single-parameter criteria are not suitable. The results also show that the strength of concrete under equal bi-axial compression is not equal to uniaxial compressive strength ($f_{cc} \neq f_c$), therefore, the three-parameter criterion is better. The two-parameter criterion of single-shear theory

(Mohr-Coulomb strength theory) and the three-parameter criterion of single-shear theory (dashed line) are plotted in Fig. 19.34. The simulated results do not match them.

The simulation results can also be fitted by using the experience curve. But the curve equation is not easy for using.

This simulation result may be matched by a three-parameter criterion reduced from the three-parameter unified strength theory. Comparison of the micromechanical analysis of concrete under plane stress with the three-parameter unified strength theory is shown in Fig. 19.35. In the figure, the dashed line is the three-parameter single-shear theory (or the three-parameter unified strength theory with $b=0$); the solid line is the three-parameter unified strength theory with $b=1$; dot dashed line is the three-parameter unified strength theory with $b=1/2$. They showed an intersection relationship between the simulated results and the three-parameter unified strength theory with $b=1/2$.

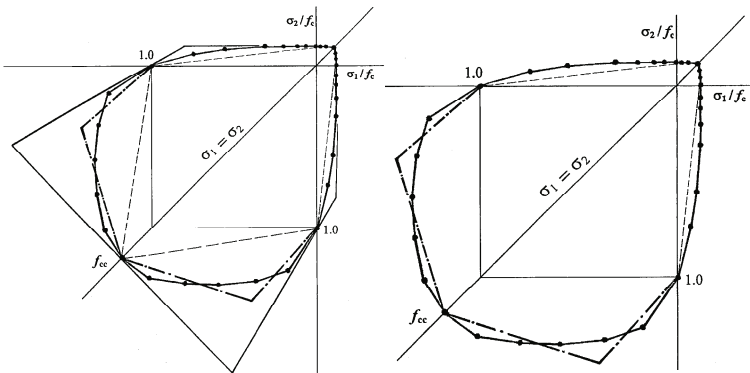


Fig. 19.35 The comparison of the micromechanical analysis of concrete under plane stress with the three-parameter unified strength theory

19.13 Brief Summary

Mesomechanics and multiscale modelling for yield surface are studied in this chapter. The prediction of strength of materials and structures for different scale yield surface is influenced strongly by the choosing of the material model. It is very important that how to choose the reasonable strength theory (yield criteria, failure criterion, or material model in FEM code) in the research and design. The change in shape and size of the yield surface of various failure criteria is great. A general, but simple and thereby suited for many potential users may be developed.

The interaction yield surface of structures, yield loci of polycrystalline aggregates under the combined stress (σ - τ) (Lin and Ito), models in meso and macro mechanics, failure surface for cellular materials under multiaxial loads, multiscale analysis of composite using UST (Li and Ishii), multiscale analysis of

yield criterion of metallic glass based on atomistic basis (Schuh and Lund), atomic-scale study of plastic-yield criterion in nanocrystalline CU (Dongare et al., 2010), multiscale analysis of yield criterion of molybdenum and tungsten based on atomistic basis (Grogger), phase transformation yield criterion of shape-memory alloys (Lexcellent et al., 2002; 2004; 2007; Gibeau, 2010; Bhattacharya and Schlömerkemper, 2004), extremal yield surfaces of a unit cell (Schrefler, 2009), damage surface under combined stress (Murakami, Hayakawa and Liu Y)), virtual material testing based on crystal plasticity finite element simulations (Roters et al., 2010) and meso-mechanical analysis of failure criterion for concrete (Liu et al., 1972; Yu and Zeng, 1993; Caballero, 2007) are described in this chapter.

A general yield criterion for unit cell in multiscale plasticity is proposed in Section 19.10, and several comparisons between yield surfaces of material in multiscale plasticity are given in Sections 19.10 and 19.12.

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