Chapter 9
Estimation of the Stress State Within Particles and Inclusions and a Nucleation Model for Particle Cracking

Despite great strides in developing physically motivated models for void growth, shape evolution and coalescence, a suitable treatment for void nucleation remains an open question. Accurate modeling of void nucleation is difficult within a Gurson-based framework due to the intrinsic assumption that the material does not contain any second-phase particles. Consequently, the nucleation models employed in these constitutive models are overly simplistic as the particle shape, composition, stress state and load-sharing are neglected, lumped into a single calibration parameter (Beremin 1981) or indirectly accounted for in a phenomenological manner (Chu and Needlman 1980). The lack of progress in developing physically sound nucleation models has not been for lack of effort but a result of the inherently complex nature of the nucleation process. Void nucleation is very difficult to capture experimentally since it is a relatively random and instantaneous event that cannot be captured in-situ without the aid of high resolution x-ray tomography. Additionally, the local stress state near a particle of interest is typically unknown, as well as the particle composition and mechanical properties. The nucleation mechanism can occur by debonding or particle cracking and is influenced by the particle size, shape, composition, distribution, strain rate and temperature. From an engineering perspective, one can clearly see the attraction in adopting a phenomenological nucleation model whose parameters can be adjusted to give good agreement with the experiment data. Nevertheless, there is ample opportunity to improve the physical foundation of the current nucleation models, especially in regards to percolation modeling.

A promising procedure to account for the stress state in the particles has been proposed by Butcher (2011) by integrating a secant-based homogenization technique for particle-reinforced plasticity into an existing damage-based material model. This model has been developed to predict ductile fracture of industrial alloys during sheet metal forming operations where the loading is proportional and the particle content is small. The subsequent sections will introduce the particle-based homogenization model and its integration into a general damage-based constitutive model. The ability to determine the stress state within the particles will be used to model nucleation in Chaps. 10 and 11.

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9.1 Particle-Based Homogenization Theories

The development of particle-based homogenization theories to predict the bulk behavior of a material from its constituents encompasses a large branch of materials mechanics. As such, only a very brief review of the development of homogenization techniques is presented here with a focus on methods amenable for implementation into a damage-based framework. Excellent reviews on the efforts to develop particle-based homogenization techniques in the plastic regime can be found in Ponte-Casteneda and Suquet (1998) and Chaboche et al. (2005).

The framework for particle-based homogenization problems was pioneered by Eshelby (1957) when he obtained closed-form solutions for the stress field within ellipsoidal inclusions embedded in a matrix material by theorizing a stress-free transformation strain (eigen-strain) between the matrix and inclusions. Eshelby's work provided the analytical techniques required to estimate the average stress within the inclusions and matrix material using his so-called fourth-order **S** tensor. Hill (1965) later developed a rigorous solution for composite materials using the incremental theory of anisotropic elasticity. Incremental approaches to the homogenization process are based upon the tangent stiffness tensors of the constituents. It was soon recognized that this approach led to overestimations in the flow stress of the material due to the anisotropic nature of the tangent stiffness tensor in the plastic regime.

To obtain more realistic predictions for the composite flow stress, Berveiller and Zaoui (1979) modified Hill's incremental solution to obtain a total-strain formulation for proportional loading using the secant moduli of the matrix material. This model was further improved by Weng (1984, 1990) and Tandon and Weng (1986) using the mean field methods of Mori and Tanaka (1973) to account for inclusion interactions. Although the experimental material behaviour was better described using these models, errors arose when the inclusions remained elastic, resulting in an overly stiff response and an overestimation of the composite flow stress. The reason for this error was attributed to the fact that the plastic strain in the matrix was determined from a reference equivalent stress using the volumetric average of the matrix stress tensor. This equivalent stress can be significantly lower than the phase-average of the equivalent stress due to the severe stress gradients that develop in the plastic regime, resulting in the composite stress to be overestimated (Pierard et al. 2007).

This limitation led to the development of a modified secant method that defines the stress field in the non-linear matrix phase using the second-order moment of the volumetric stress tensor by Suquet (1995). The modified secant approach coincides with the variational approach of Ponte Castenada (1996) and gives very good agreement with the finite-element solution for a ductile matrix embedded with spherical elastic inclusions (Segurado, J., & Llorca, J. 2002). Despite these improvements, a fundamental limitation of secant-based methods is that they cannot be applied for non-proportional loadings, resulting in a renewed interest in recent years to improve the incremental formulations. Significant improvements have been obtained in the incremental models by using only the isotropic component of the anisotropic tangent stiffness tensors (Gonzalez and Llorca 2000; Doghri and Ouaar 2003).

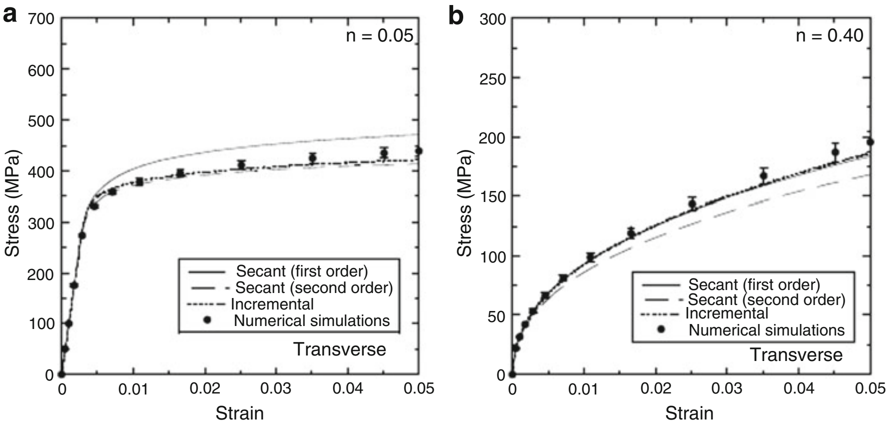

Fig. 9.1 Predictions of the tensile stress–strain curves in the longitudinal direction for the composite reinforced with ellipsoidal inclusions with a volume fraction of 25 %. (**a**) n = 0.05; (**b**) n = 0.40. The error bars represent the standard deviation in the numerical simulations (Reprinted with permission from Pierard et al. (2007). Copyright 2007 Elsevier)

Today, it is generally agreed that both secant and tangent-based homogenization models can provide acceptable approximations to the material behavior of composite materials in the elastic and plastic regimes (Pierard et al. 2007). As each type of model has its advantages, the desired application of the model is perhaps the most important factor in its selection. For materials with dilute concentrations of inclusions (less than 10 %), Mueller and Mortensen (2006) found no discernible difference in the predictions for the bulk and shear moduli of the composite when they evaluated five different homogenization schemes in the plastic regime (secant, self-consistent, generalized self-consistent, differential effective-medium, identical hard spheres approximation). This result suggests that a simple homogenization model can be suitable for a large range of engineering alloys.

A recent work by Pierard et al. (2007) provides additional insight into the importance of selecting the appropriate homogenization scheme. In this work, a finite-element study was conducted for a material containing aligned ellipsoidal inclusions to obtain an 'exact' solution to the homogenization problem. A classical secant (Mori and Tanaka 1973), modified secant (Suquet 1997) and a modified incremental model (Doghri and Ouaar 2003) were then evaluated to measure their predictive abilities. It was observed that the modified secant method gave the best agreement with the numerical results at the onset of plastic deformation while the classical method gave the best prediction for the composite hardening rate in the fully plastic regime. The incremental model of Doghri and Ouaar (2003) provided very good results in all of the cases considered. A comparison of the results with the 'exact solution' obtained using finite-element simulations is shown in Fig. 9.1.

What is most interesting from the work of Pierard et al. (2007) with respect to void nucleation is that while the incremental and modified secant methods gave the best estimates for the composite stress, the stress within the particles was best predicted using the secant method shown in Fig. 9.2. This is an important result and

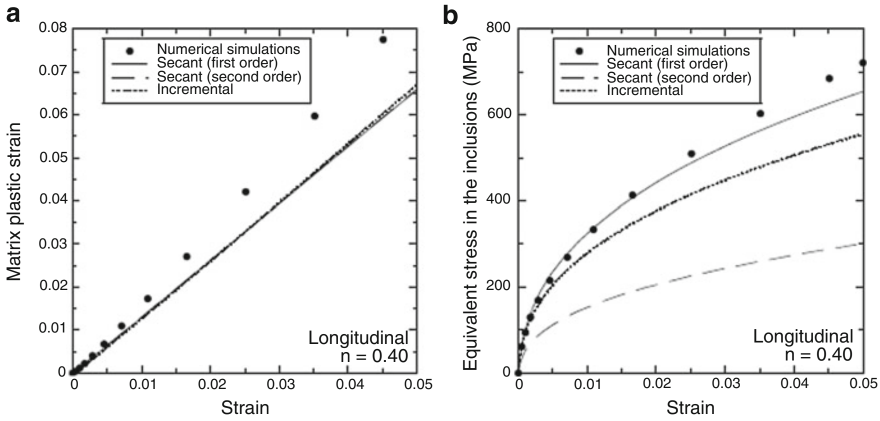

Fig. 9.2 (**a**) Evolution of the plastic strain in the matrix as a function of the applied strain. (**b**) Evolution of the von Mises equivalent stress in the ellipsoids as a function of the applied strain. The composite was loaded in the longitudinal direction and the matrix hardening coefficient was 0.40 (Reprinted with permission from Pierard et al. (2007). Copyright 2007 Elsevier)

it emphasizes the fact that that the ability of a model to predict the overall response of a material from its constituents does not mean that the predicted stress within the constituents is accurate as well. It is also important to note that all of the models underestimated the plastic strain in the matrix as the strong strain-gradients that develop between inclusions are not captured. These results serve to highlight the approximate nature of the homogenization models and one can see that in many cases, there may not be a distinct advantage in selecting one model over the other. The specific application and degree of accuracy in the metric of interest should be used in selecting an appropriate model.

9.2 Selection of a Homogenization Theory for Modelling Void Nucleation

For many ductile industrial alloys the volume fraction of second-phase particles is on the order of a few percent. As such, the reinforcement of these particles on the stress–strain curve is not of prime concern since they are generally not considered at all in Gurson-based material models. The influence of the particles in Gurson-based models is implicitly captured by using the experimental flow stress relation and assuming it describes the behaviour of the 'virgin' matrix. Consequently, our objective is to augment existing damage-based constitutive models by improving their ability to predict void nucleation through knowledge of the stress within the inclusions, not to predict the macroscopic response of the material from homogenization theory. The initiation and evolution of voids is the principal concern. If the material of interest contains a large volume fraction of reinforcing particles, a sophisticated homogenization scheme may be required to predict the overall response of the material to capture the load loss as particles nucleate voids.

For the purpose of modeling void nucleation, the secant method of Tandon and Weng (1986) will be used to estimate the stress within the inclusions. The advantages of adopting a secant-based method are that they are computationally efficient, easily implemented into numerical codes and can provide reasonable estimations for the stress in the matrix and inclusions. The issue of computational efficiency is of paramount importance in a damage percolation model because the homogenization procedure must be repeated for each of the large number of particles within the microstructure at each loading step. The adoption of a more sophisticated homogenization model is left for future work.

9.3 A Particle-Based Homogenization Model for a Dual-Phase Composite Subjected to a Prescribed Traction

The particle-based homogenization scheme considered in this work was developed by Tandon and Weng (1986) for a dual-phase composite subjected to a prescribed traction. The composite is composed of three-dimensional, randomly oriented elastic particles embedded within a ductile matrix. The particles are spheroidal and characterized by their elastic properties, volume fraction and aspect ratio. The homogenization theory is valid for inclusion shapes ranging from flat discs, to ellipsoids, to elongated fibres.

The homogenization model of Tandon and Weng (1986) is a secant-based approach that utilizes Berveiller and Zaoui's (1979) modification to the solution of Hill (1965) for proportional loading and incorporates the mean-field method of Mori and Tanaka (1973) to account for particle interactions. Additional details of the derivation of this model can be found in Tandon and Weng (1986). The following section will present the details of this theory relevant for integration with a damage-based constitutive model.

9.4 Effective Moduli of a Randomly-Oriented Composite

The ductile matrix material is treated as phase 0 and the embedded elastic particles are defined as phase 1 with a volume fraction, f_1, and aspect ratio, W_1. The respective isotropic Poisson's ratio, and bulk, shear and elastic moduli of the r-th phase are denoted by ν_{r}, κ_{r}, μ_{r} and $\mathrm{E_r}$ with a superscript, s, used to denote a secant quantity such as the secant shear modulus of the matrix, μ_0^s. The stress and strain tensors for the r-th phase are denoted by $\sigma_{ij}^{(r)}$ and $\varepsilon_{ij}^{(r)}$ which can be decomposed into their respective deviatoric and hydrostatic components as $\sigma_{ij}^{(r)} = \sigma_{ij}^{('r)} + \delta_{ij}\sigma_{\mathrm{hyd}}^{(r)}$ with

$\sigma_{\mathrm{hyd}}^{(r)} = \sigma_{kk}^{(r)}/3$ and $\varepsilon_{ij}^{(r)} = \varepsilon_{ij}^{(r)} + \delta_{ij}\varepsilon_{\mathrm{hyd}}^{(r)}$ with $\varepsilon_{\mathrm{hyd}}^{(r)} = \varepsilon_{kk}^{(r)}/3$ where δ_{ij} is the Kronecker delta. Any property or quantity associated with the composite is denoted using an overbar symbol such as $\bar{\sigma}_{ij}$ for the composite stress tensor.

In a composite material the constituents are generally in a triaxial state of stress that should be characterized using the equivalent measures for the stress, strain and plastic strain as

$$\sigma_{\mathrm{eq}}^{(r)} = \sqrt{(3/2)\sigma_{ij}^{('r)}\sigma_{ij}^{('r)}} \qquad \varepsilon_{\mathrm{eq}}^{(r)} = \sqrt{(2/3)\varepsilon_{ij}^{('r)}\varepsilon_{ij}^{('r)}}$$
$$\bar{\varepsilon}_{\mathrm{eq}}^{\mathrm{p}} = \sqrt{(2/3)\bar{\varepsilon}_{ij}^{\mathrm{p}}\bar{\varepsilon}_{ij}^{\mathrm{p}}} \tag{9.1a, b, c}$$

The components of the stress and strain in the composite are related through the effective secant shear and bulk moduli as

$$\bar{\sigma}_{ij}^{'} = 2\bar{\mu}^{s}\bar{\varepsilon}_{ij}^{'} \qquad \bar{\sigma}_{\mathrm{hyd}} = 3\bar{\kappa}^{s}\bar{\varepsilon}_{\mathrm{hyd}} \tag{9.2a, b}$$

To determine the stress and strain in the composite and its constituents during plastic deformation, the effective secant elastic moduli of the matrix and composite must first be determined as functions of the matrix plastic strain, $\varepsilon_{\mathrm{eq}}^{\mathrm{p}(0)}$. The secant elastic modulus and Poisson's ratio of the matrix are expressed as

$$\mathrm{E}_0^{s} = \frac{1}{\frac{1}{\mathrm{E}_0} + \frac{\varepsilon_{\mathrm{eq}}^{\mathrm{p}(0)}}{\sigma_{\mathrm{eq}}^{(0)}}} = \frac{3\mathrm{E}_0\mu_0^{s}}{\mathrm{E}_0 + \mu_0^{s}(1-2\nu_0)} \qquad \nu_0^{s} = \frac{1}{2} - \left(\frac{1}{2} - \nu_0\right)\frac{E_0^{s}}{E_0} \tag{9.3, 9.4}$$

The secant bulk and shear moduli are obtained using the standard isotropic relations $\mu_0^{s} = \mathrm{E}_0^{s}/2(1+\nu_0^{s})$ and $\kappa_0^{s} = \mathrm{E}_0^{s}/3(1-2\nu_0^{s})$. The matrix material is assumed to be plastically incompressible and thus the secant bulk modulus remains constant at $\kappa_0^{s} = \kappa_0$. The effective secant moduli of the composite material can be determined as

$$\bar{\kappa}^{s} = \frac{\kappa_0}{(1+f_1 p_{2s}/p_{1s})} \qquad \bar{\mu}^{s} = \frac{\mu_0^{s}}{(1+f_1 q_{2s}/q_{1s})} \tag{9.5, 9.6}$$

where p_{is} and q_{is} are functions of the particle shape, volume fraction, elastic moduli of the constituents and the fourth-order Eshelby (1957) **S** tensor. The expressions for p_{is} and q_{is} are rather lengthy and are not presented here for brevity but can be found in Tandon and Weng (1986).

9.5 Average Stress in the Composite and Its Constituents

The respective hydrostatic and deviatoric stresses in each constituent are determined from the composite stress tensor using the stress concentration factors, $a^{(r)}$ and $b^{(r)}$ as

$$\sigma_{\mathrm{hyd}}^{(r)} = a^{(r)}\bar{\sigma}_{\mathrm{hyd}} \qquad \sigma_{ij}^{('r)} = b^{(r)}\bar{\sigma}'_{ij} \qquad \sigma_{eq}^{(r)} = b^{(r)}\bar{\sigma}_{eq} \tag{9.7a, b, c}$$

that are defined for the matrix material and particles as

$$a^{(0)} = 1/p_{1s} \qquad a^{(1)} = \left(1 - (1-f_1)a^{(0)}\right)/f_1 \tag{9.8a, b}$$

$$b^{(0)} = 1/q_{1s} \qquad b^{(1)} = \left(1 - (1-f_1)b^{(0)}\right)/f_1 \tag{9.9a, b}$$

The stress in the composite and its constituents must be in equilibrium and thus

$$\bar{\sigma}_{ij} = (1-f_1)\sigma_{ij}^{(0)} + f_1\sigma_{ij}^{(1)} \tag{9.10}$$

The onset of yielding of the matrix occurs when $\bar{\sigma}_{\mathrm{eq}} \geq \sigma_{\mathrm{y}}^{(0)}/b^{(0)}$ with $b^{(0)}$ determined using the elastic moduli of the matrix in Eq. (9.3) and (9.4).

9.6 Average Strain in the Composite and Its Constituents

Due to the presence of the elastic inclusions, the composite is not plastically incompressible and the composite plastic strain must be determined from the unloading process as

$$\bar{\varepsilon}_{ij}^{\mathrm{p}} = \left(\frac{1}{2\bar{\mu}_s} - \frac{1}{2\bar{\mu}}\right)\bar{\sigma}'_{ij} + \delta_{ij}\left(\frac{1}{3\bar{\kappa}_s} - \frac{1}{3\bar{\kappa}}\right)\bar{\sigma}_{\mathrm{hyd}} \tag{9.11}$$

The matrix is assumed to be isotropic and obey J_2 plasticity (von Mises material) from which the plastic strain components can be readily determined by integrating the J_2 flow rule for proportional loading to yield

$$\varepsilon_{ij}^{\mathrm{p}(0)} = \frac{3}{2}\frac{\varepsilon_{\mathrm{eq}}^{\mathrm{p}(0)}}{\bar{\sigma}}\bar{\sigma}'_{ij} \tag{9.12}$$

The particles are assumed to remain elastic during deformation and the strain in the particles can be expressed as

$$\varepsilon_{ij}^{(1)} = \frac{b^{(1)}\bar{\sigma}_{ij}'}{2\mu_1} + \delta_{ij}\frac{a^{(1)}\bar{\sigma}_{\text{hyd}}}{3\kappa_1} \tag{9.13}$$

The solution for the secant moduli of the composite and subsequent stress and strain in the constituents is nonlinear and an iterative solution is required in the plastic regime. The required material parameters to determine the behaviour of the composite and stress in the constituents are E_0, ν_0, E_1, ν_1, f_1, and W_1. A simple fixed-point algorithm can be easily implemented to determine the required value for $\varepsilon_{\text{eq}}^{\text{p}(0)}$ and is described in Tandon and Weng (1986). However, this solution method must be modified in the present work because the homogenization method is to be coupled with a damage-based constitutive model to account for the influence of voids on the subsequent stress and strain in the constituents.

9.7 Procedure for Integrating a Particle-Based Homogenization Theory into an Existing Damage-Based Constitutive Model

To integrate a particle-based homogenization theory into a damage-based constitutive model, we assume that the bulk material can be idealized as a three-phase composite composed of a matrix material with embedded particles and voids. It is assumed that this idealized three-phase composite can be decomposed into its constituents by applying two successive homogenization schemes: (i) a Gurson-based constitutive model for the voids embedded in a ductile 'composite matrix' which is composed of the particles and matrix material and (ii) separation of the composite matrix into its constituents to determine the stress within the matrix and particles using a secant-based homogenization scheme.

Let us consider a bulk material which contains both voids and hard elastic particles/inclusions within a ductile matrix. To mitigate the influence of the voids, the experimental flow stress relation for the bulk material can be obtained from a torsion or compression-type test or from a tensile test if the initial porosity is negligible (Pardoen 2006). This flow stress relation is essentially that of a two-phase composite composed of the matrix and particles.

Now, the bulk material is subjected to a deformation process such as a sheet metal forming operation where the pre-existing voids will grow and additional voids will be nucleated from particle cracking and/or debonding from the matrix. The presence of the voids results in material softening which further promotes void evolution resulting in ductile fracture as the voids coalesce and link-up throughout the material. The influence of the voids on the response of the bulk material can be described using a damage-based constitutive model such as the Gurson (1977) model. Gurson-based models are the result of a homogenization procedure for a material composed of voids embedded within a virgin matrix. Therefore, a Gurson-based model can be applied to the bulk material to account for void damage by modeling the bulk material as a material which contains voids embedded within a so-called composite matrix. The composite matrix is composed of the virgin matrix and particles whose composite behaviour is described using the experimental flow-stress relation for a two-phase composite as described above.

The typical procedure for the integration of the Gurson-based material model is now applied to the bulk material. The material has a void volume fraction or porosity, f, and is subjected to a monotonic proportional loading with a macroscopic strain, $\bar{E}_{ij}$. The stress state is then integrated using the damage-based yield surface to determine the macroscopic stress, Σ_{ij}. The equivalent plastic strain and flow stress within the composite matrix are, $\bar{E}^{\mathrm{p}}_{\mathrm{eq}}$ and $\bar{\sigma} = \bar{\sigma}(\bar{E}^{\mathrm{p}}_{\mathrm{eq}})$. Void evolution is very sensitive to the stress state which is characterized by the stress triaxiality ratio defined as $T = \bar{\Sigma}_{\mathrm{hyd}}/\bar{\Sigma}_{\mathrm{eq}}$.

Due to the presence of the voids, the bulk material is softer and thus the composite matrix must work-harden to a greater extent to reach the applied strain of $\bar{E}_{ij}$ than if no voids were present. Since the voids do not contribute to load-sharing, the entire stress must be borne by the matrix and particles. Therefore, from the perspective of the constituents, it is equivalent to subjecting the composite matrix to a larger applied strain denoted $\bar{\varepsilon}_{ij}$, that results in the same equivalent stress and plastic strain as when softening was considered.

The situation for the composite matrix now resembles that of a particle-based homogenization problem for a prescribed traction. The equivalent stress state within the composite matrix is known and the stress state in the constituents must be determined that is in equilibrium with this prescribed stress. The secant-based homogenization method of Tandon and Weng (1986) can now be applied to determine the effective secant moduli of the composite matrix which satisfy the stress state defined by the damage-based stress integration.

The general integration procedure is presented in Fig. 9.3 and can be summarized in the following steps:

(a) A bulk material containing voids and particles within a ductile matrix is subjected to a macroscopic loading.
(b) The voids within the material are homogenized into an equivalent void embedded in a composite matrix.
(c) The material is now that of a Gurson-based material with the composite matrix taking the place of the virgin matrix
(d) A damage-based constitutive model is applied to determine the stress in the composite matrix by accounting for the influence of the voids. This decouples the void from the composite matrix.
(e) With the voids removed from the composite matrix, a particle-based homogenization theory for a prescribed traction is applied to the composite matrix to determine the stress within the matrix and particles.
(f) The particles can now be tested for nucleation using an appropriate model for the material.
(g) The evolution of the voids must obey the plasticity of the matrix. Combine the isolated void and the virgin matrix to obtain the traditional voided unit cell.

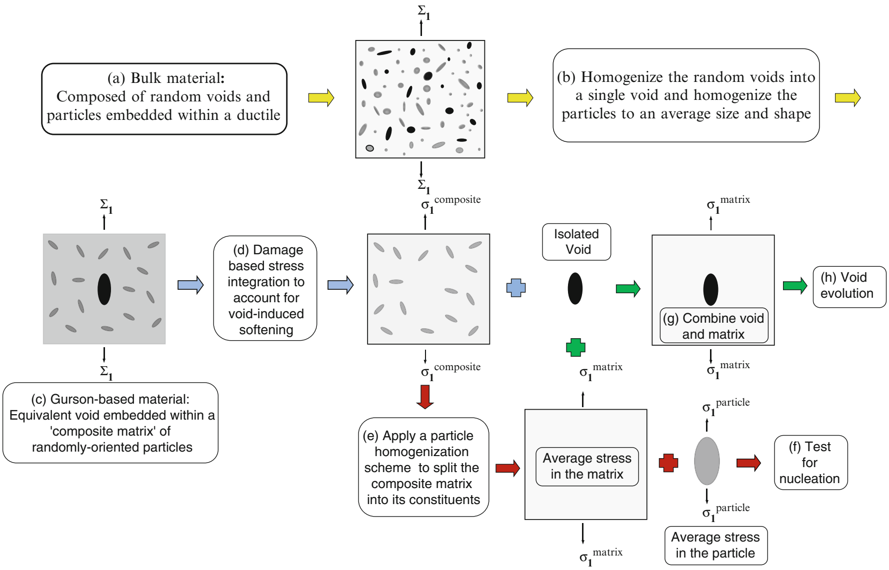

Fig. 9.3 Schematic of the integration process of a particle-based homogenization theory into a damage-based constitutive model (Butcher 2011)

(h) The standard models for void evolution are evaluated using the stress state and plastic strain of the matrix.

To create a stress state in the composite matrix equivalent to that of the voided bulk material, the applied strain, $\bar{\varepsilon}_{ij}$, must be determined to produce a stress, $\bar{\sigma}_{ij}$, subject to the constraints that $\bar{\sigma}_{eq} = \bar{\sigma}$, $\bar{\varepsilon}^{p}_{eq} = \bar{E}^{p}_{eq}$ and $\bar{\sigma}_{hyd}/\bar{\sigma}_{eq} = T$. It is important to mention that the equivalent stress, Σ_{eq}, identified in the damage-based integration is not equal to the flow stress within the composite matrix due to the presence of the voids. The procedure to determine the applied strain, $\bar{\varepsilon}_{ij}$, and stress, $\bar{\sigma}_{ij}$, within the composite matrix using a secant-based homogenization scheme for monotonic, proportional loading is described in the following section.

First, the hydrostatic stress of the composite matrix can be computed directly from the requirement of an equivalent triaxiality as

$$\bar{\sigma}_{hyd} = \bar{\sigma}(\bar{\Sigma}_{hyd}/\bar{\Sigma}_{eq}) \tag{9.14}$$

From the definition of the effective secant moduli in Eq. (9.2) and the equivalent stress and strain in Eq. (9.1a, b), the equivalent strain in the composite matrix is

$$\bar{\varepsilon}_{eq} = \bar{\sigma}/3\bar{\mu}^{s} \tag{9.15}$$

Only the deviatoric stress and strain of the composite matrix remain unknown and only one is required to be pre-determined as they are related through the secant shear modulus. The deviatoric strain in the composite is assumed to be proportional to the deviatoric strain in the damage-based model or three-phase composite as

$$\bar{\varepsilon}_{ij}^{'} = \xi \bar{E}_{ij}^{'} \tag{9.16}$$

so that $\xi = \bar{\varepsilon}_{\text{eq}} / \bar{E}_{\text{eq}}$, and the stress and applied strain in the composite matrix can be derived as

$$\bar{\sigma}_{ij} = \left(\frac{2}{3} \frac{\bar{\sigma}}{\bar{E}_{\text{eq}}} \right) \bar{E}_{ij}^{'} + \delta_{ij} \bar{\sigma}_{\text{hyd}} \qquad \bar{\varepsilon}_{ij} = \left(\frac{1}{3\bar{\mu}^s} \frac{\bar{\sigma}}{\bar{E}_{\text{eq}}^{\text{p}}} \right) \bar{E}_{ij}^{'} + \delta_{ij} \frac{\bar{\sigma}_{\text{hyd}}}{3\bar{\kappa}^s} \tag{9.17, 9.18}$$

which satisfies the requirements that $\bar{\sigma}_{\text{hyd}} / \bar{\sigma}_{\text{eq}} = T$ and $\bar{\sigma}_{\text{eq}} = \bar{\sigma}$. The stress within the composite matrix can be evaluated immediately following the stress integration of the damage-based constitutive model while $\bar{\varepsilon}_{ij}$ requires knowledge of the effective secant moduli which have yet to be determined.

9.8 Iterative Solution for the Effective Secant Moduli

An iterative procedure is required to determine the effective secant moduli of the composite matrix from which the stress and strain within the constituents can be determined. The iterative solution is developed through the final constraint that the secant elastic moduli must result in a plastic strain in the composite matrix of $\bar{\varepsilon}_{\text{eq}}^{\text{p}} = \bar{E}_{\text{eq}}^{\text{p}}$. The plastic strain of the composite matrix must account for the elastic heterogeneity of the particles and from substituting Eq. (9.11) into Eq. (9.2) and utilizing Eq. (9.1c), the required secant shear modulus of the composite matrix is

$$\bar{\mu}^{s*} = \bar{\mu}\bar{\sigma} \left(\bar{\sigma} + \bar{\mu} \sqrt{\left(3\bar{E}_{\text{eq}}^{\text{p}}\right)^2 - 2\left(1/\bar{\kappa}^s - 1/\bar{\kappa}\right)^2 \bar{\sigma}_{\text{hyd}}^2} \right)^{-1} \tag{9.19}$$

All of the parameters in Eq. (9.19) are constant during the iteration loop except for the secant bulk modulus, $\bar{\kappa}^s$, which varies with the plastic strain of the matrix.

A fixed-point algorithm is used to obtain the solution to the non-linear equations for the secant moduli by iterating upon the secant elastic modulus of the matrix, E_0^s. A trial value for E_0^s is assumed from which the subsequent trial values for the secant shear, bulk and Poisson's ratios of the matrix can be determined from Eqs. (9.3) and (9.4) and used to evaluate the expressions for p_{is} and q_{is}, as well as $\bar{\kappa}_s$ in Eq. (9.5) and $\bar{\mu}^{s*}$ in Eq. (9.19). A new estimate for μ_0^s can be determined by setting $\bar{\mu}^s = \bar{\mu}^{s*}$ in Eq. (9.6) and evaluating Eq. (9.3) to obtain a new estimate for E_0^s. If this new value of E_0^s is equal to the trial value, the solution has been obtained, otherwise the algorithm is repeated using the current E_0^s as the new trial value. Upon convergence, the stress concentration factors to determine the stress and strain tensors of the matrix and particles can be evaluated using Eqs. (9.7a–c), (9.12) and (9.13). This algorithm generally achieves convergence within three iterations to a tolerance of 0.001 and is straightforward in its implementation.

9.9 Application of the Particle-Based Homogenization Scheme into a Gurson-Based Constitutive Model for Ductile Fracture

The integration of a homogenization scheme into a Gurson-based damage framework improves all aspects of the damage model and couples the various damage mechanisms that are often considered independently. The advantages of the proposed fully-coupled damage-based constitutive model are:

- Modeling of void nucleation is improved through knowledge of the stress state within the particles as a function of their shape, content and composition.
- As particles nucleate voids, the stress state within the matrix becomes more severe due to increased material softening (higher porosity) as fewer particles are available for load sharing.
- The stress state within the matrix and particles becomes progressively more severe as the particle content decreases due to nucleation. This promotes additional nucleation, void growth and material softening.
- The plastic strain within the matrix material is higher than in the composite matrix and thus promotes void evolution and coalescence.
- The model reverts to its original formulation if the material does not contain any second-phase particles or inclusions.
- The flow stress relation of the matrix material does not have to be predetermined.
- An absolute minimum number of new parameters have been introduced into the damage-based framework. The elastic properties of the constituents as well as the average particle shape and content are typically known from standard material characterization techniques used in damage-based modeling.
- The particle-based homogenization scheme is computationally efficient and easily implemented into any existing damage-based constitutive model.

The proposed integration procedure has been implemented into the well-known GT constitutive model in Butcher (2011) and is also used in the percolation model by applying the homogenization procedure to each particle in the material. The variation in the principal stress state in the particles with the macroscopic stress state is shown in Fig. 9.4.

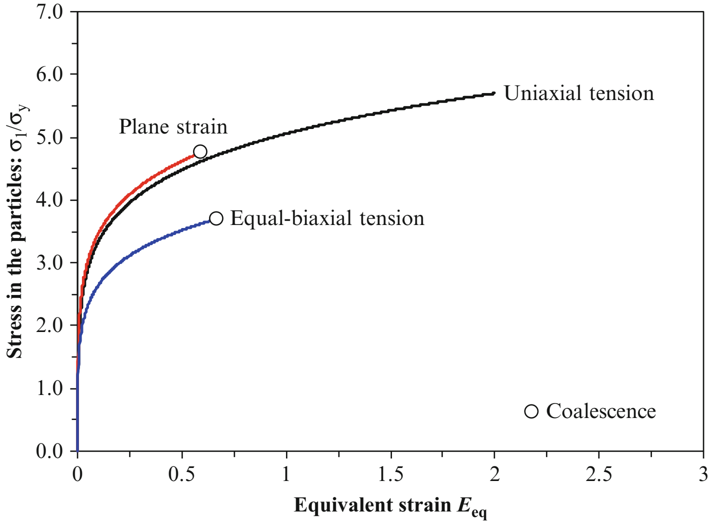

Fig. 9.4 Normalized principal stress within the spherical elastic particles/inclusions with a volume fraction of 10 % for three loading conditions in a model material based upon AA5083 (Butcher 2011). The initial voids in the material have an aspect ratio of 1/6 and a porosity of 0.1 %. The bulk material ruptures due to void coalescence when loaded in plane strain and equal-biaxial tension

9.10 Continuum Nucleation

The treatment of void nucleation on the continuum scale in a damage-framework can be substantially improved using the the proposed integration scheme to obtain the stress in the particles. For example, the nucleation stress in the Chu and Needleman (1980) nucleation model can now be predicted as a function of the particle content, shape and elastic moduli as

$$\dot{f}_{\text{nucleation}}(f_p, W_p, G_p, \kappa_p, \Sigma_{ij}) = \frac{W_{\text{N}}\xi_{\text{n}}f_{\text{p}}}{s_{\text{N}}\sigma_{\text{y}}\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\sigma^p - \sigma_{\text{N}}}{s_{\text{N}}\sigma_{\text{y}}}\right)^2\right]\dot{\sigma}^p \tag{9.20}$$

where W_{N} is the aspect ratio of the nucleated void and ξ_{n} is the fraction of particles that will nucleate voids. The particle stress term, σ_{p}, can be either the equivalent stress in the particles for general nucleation modelling or the maximum principal stress in the particles to better represent particle cracking. The yield stress of the material, σ_{y}, is simply a normalizing factor and could be changed to the particle yield stress if it happens to be known. Unlike the traditional Chu and Needleman nucleation model (1980), the stress in the particles will evolve as particles nucleate voids, increasing the stress in the remaining particles and promoting nucleation. Furthermore, the determination of the mean nucleation stress, σ_{N}, through calibration with the experiment will have a stronger physical foundation since the stress in the particles was determined as a function of the global stress state and the particle morphology.

9.11 Void Nucleation in a Particle Field

The dominant void nucleation mechanisms in ductile materials are particle cracking and interface fracture (debonding). Particle cracking occurs primarily in strong, rigid particles in a brittle-type fracture in the direction transverse to the maximum principal stress. Void nucleation due to interface separation is strongly related to the particle geometry and the interface strength between the inclusion and the surrounding matrix. Similar to particle cracking, debonding occurs preferentially in the principal loading direction unless the stress triaxiality is high.

From a modeling perspective, particle cracking and debonding will occur simultaneously in a material and thus two nucleation models and their parameters must be determined for each type of inclusion present. The identification of the appropriate material parameters for even a single nucleation model is a complicated process as nucleation is exceptionally difficult to measure experimentally. Consequently, most treatments of nucleation rely on a phenomenological model such as a normal-distribution (Chu and Needleman 1980) with either assumed or calibrated parameters obtained from a combination of finite-element simulations and experiment data (Butcher and Chen 2011).

In a damage percolation model, an approximate treatment for nucleation is required to reduce the number of required nucleation parameters while retaining a physically sound description of the nucleation mechanism. A proper accounting of nucleation requires both a nucleation model and a treatment for determining the initial dimensions and orientation of the nucleated void. For practical considerations, an emphasis is placed upon developing an accurate representation of particle cracking as this is the dominant nucleation mode in many advanced automotive alloys. Additionally, the nucleated void by particle cracking gives rise to a penny-shaped void whose growth and evolution is relatively well understood from finite-element simulations in Chap. 4. The implementation of a sophisticated particle debonding criterion into the percolation framework is left for future work.

9.12 Modeling Void Nucleation Using Penny-Shaped Voids

In particle cracking, the void is assumed to nucleate transversely to the maximum principal direction as illustrated in Fig. 9.5. This cracking behaviour is similar for both oblate and prolate ellipsoidal inclusions with prolate inclusions particularly prone to cracking. At the instant of nucleation, the particle is in two pieces that have yet to appreciably separate and the void is said to be penny-shaped. From unit cell simulations of penny-shaped voids, it has been shown that the growth of the void and response of the material converges for aspect ratios lower than 1/100. This is an extremely beneficial result that allows us to assume an aspect ratio for the nucleated void with the confidence that is a physically sound approximation.

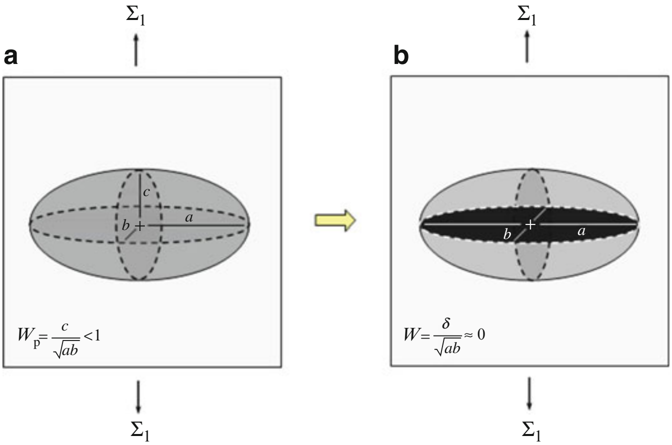

Fig. 9.5 Void nucleation by the cracking of an oblate ellipsoidal inclusion. Nucleation occurs in the same manner for a prolate ellipsoid. (**a**) Oblate ellipsoidal particle or inclusion and (**b**) particle cracks to form a penny shaped void

For particle debonding, we will first consider an oblate ellipsoidal particle as viewed from the principal loading direction (the particle would appear as a prolate ellipsoidal if viewed from the transverse direction). The interface may fracture at the top and/or bottom surfaces of the inclusion. At the onset of interface fracture, the vertical height of the debonded void, δ, is negligible and we assume nucleation occurs over the entire top/bottom surface. Since it is not possible to estimate whether the top and/or the bottom interface will debond first, we can take the average of the three possible cases and simply place the void at the center of the particle. As shown in Fig. 9.6, this approximation yields a penny-shaped void and can receive the same treatment for particle cracking to provide a good estimate for the initial void dimensions.

For the debonding of a prolate ellipsoidal inclusion, interface separation occurs at the top and/or bottom poles of the inclusion as shown in Fig. 9.7. Similar to the oblate inclusion, the debonded regions can be approximated by a penny-shaped void at the centroid of the inclusion.

This type of debonding is not as well represented using this treatment compared to debonding of the oblate inclusion. However, this approximation is not entirely unreasonable if it is assumed that sufficient material debonds at the pole so that the cross-sectional area of the inclusion is a good estimate for the debonded area. Nevertheless, the approximation of all nucleated voids as penny-shaped voids sufficiently covers the range of nucleation modes to be an effective and straightforward treatment as only one nucleation model is required per inclusion type. This nucleation treatment can be considered as 'cracking-centric' since it best represents particle cracking and is only approximate for debonding.

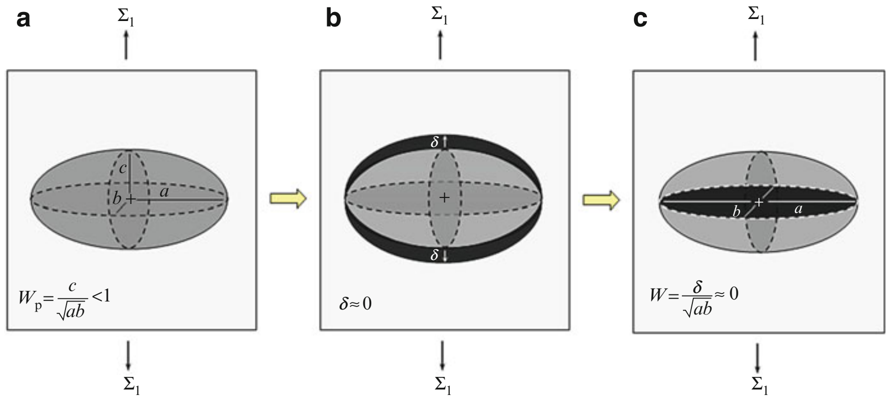

Fig. 9.6 Void nucleation by the debonding of an oblate ellipsoidal inclusion and its approximation as a penny-shaped void. (**a**) Oblate ellipsoidal particle or inclusion, (**b**) debonding may occur at the *top* and/or *bottom* surfaces of the particle, and (**c**) debonded regions approximated as a penny-shaped void at the particle centroid

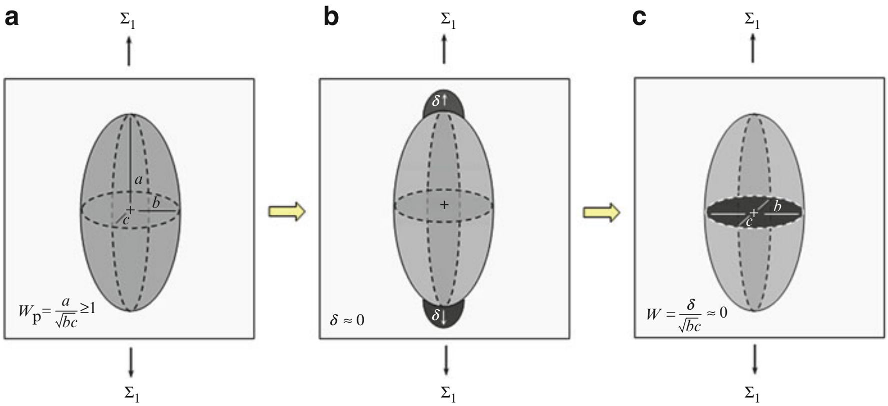

Fig. 9.7 Void nucleation by the debonding of a prolate ellipsoidal inclusion and its approximation as a penny-shaped void. (**a**) Prolate ellipsoidal particle or inclusion. (**b**) Debonding may occur at the *top* and/or *bottom* poles of the particle. (**c**) Debonded regions approximated as a penny-shaped void at the particle centroid

9.13 A Nucleation Model for Particle Cracking

A void nucleation model for particle cracking is fundamentally a model of brittle fracture and must account for the stress within the particle, particle size, shape and composition. It is well known that hard large particles are predisposed to cracking since they are irregularly shaped and experience higher stresses via load sharing with the matrix compared to their smaller neighbours. From a statistical perspective, a large particle has a higher probability of containing internal defects than a smaller particle. This effect can be clearly seen in the SEM micrographs in Fig. 9.8 that show the presence of surface cracks on the particles in an as cast AA5182 alloy.

Fig. 9.8 SEM observation from Moulin et al. (2009) showing the intermetallic particles in as-cast AA5182 (*left*) and the typical morphology of the large Fe-rich particles (*right*) (Reprinted with permission from Moulin et al. (2009). Copyright 2009 John Wiley & Sons)

These cracks are a result of the solidification process and act as preferential sites for particle break-up during the hot and cold rolling processes. In a metal forming operation, these particles are smaller but still contain cracks that can nucleate voids. Since brittle fracture is associated with negligible plastic deformation, the particles can be assumed to remain elastic during the deformation process, enabling the use of linear elastic fracture mechanics to relate the stress state with the distribution of internal cracks within the inclusions.

To model the break-up of the large intermetallic particles in AA5182 during the rolling process, Moulin et al. (2009) performed an extensive finite-element and experimental study of irregularly shaped inclusions. It was observed that the stress distribution within these particles is not homogeneous and that only certain regions of the particle will achieve the stress required for particle break-up. These high stress regions were termed the 'active volume' of the inclusion, V_a. Since the particles are brittle and contain cracks, the fracture mechanism is one of mode I failure and is a function of the critical material toughness, K_{1C}, and the distribution of the cracks. Assuming a homogeneous distribution of cracks with an effective length, a_{eff}, the crack will propagate according to Griffith's criterion for mode I fracture when the principal stress in the particle satisfies the inequality

$$\sigma_1^P \geq \frac{K_{1C}}{\sqrt{\pi a_{eff}}} \tag{9.21}$$

This equation originates from the energy requirement that the stored elastic energy within the inclusion must satisfy the energy released by the creation of the two fracture surfaces. By assuming a homogenous distribution of cracks, the inclusion is expected to contain a crack that is perpendicular to the principal loading direction that can propagate to cause fracture. The critical length of this crack, a_c, that must be present within the active volume of the inclusion can be estimated as

$$a_c \approx \frac{\alpha}{\pi}\left(\frac{K_{1C}}{\sigma_{th}}\right)^2 \qquad \alpha \approx 1 \tag{9.22}$$

where α is a geometry parameter to account for various effects such as crack blunting and interactions and σ_{th} is a threshold stress for the maximum principal stress within the active volume. The critical volume that contains a crack transverse to the loading direction is defined as $V_c^3 = a_c^3$ and particle fracture will occur when the critical volume is equal to the active volume (Moulin et al. 2009)

$$V_a \geq V_c \geq \left(\frac{\alpha}{\pi}\right)^3\left(\frac{K_{1C}}{\sigma_{th}}\right)^6 \tag{9.23}$$

9.13.1 Stress State and Nucleation

The criterion of Moulin et al. (2009) in Eq. (9.23) is ideally suited for the modeling of void nucleation since it is a volume-based metric that accounts for the stress within the inclusion, the material toughness and has a strong physical foundation based upon the energy required for crack propagation via the Griffith criterion. However, the model cannot be readily implemented into the percolation model because the threshold stress and active volume of the particles are functions of the particle size, shape, composition and loading condition. In Moulin et al. (2009), they were determined by using finite-element techniques.

Fortunately, since the inclusions in the percolation model are assumed to be ellipsoidal, the stress and strain distributions within the inclusion are uniform as proven by Eshelby (1957). This favourable result indicates that the activated volume in Eq. (9.23) must be equal to the volume of the inclusion and that the threshold stress must be equal to the principal stress in the inclusion. The homogenization scheme for particle-reinforced plasticity is now used to determine the stress within the particle as a function of the particle size, shape and composition. The fracture criterion can now be expressed in terms of a nucleation stress

$$\sigma_1^{\mathrm{p}} \geq \sigma_N \tag{9.24}$$

$$\sigma_N = \frac{1}{\sqrt{\pi}}\frac{K_{1C}^*}{V_p^{1/6}} \qquad K_{1C}^* = K_{1C}\sqrt{\alpha} \qquad \alpha \approx 1$$

where K_{1C}^* is the effective critical toughness of the particle material and is the sole parameter in the nucleation model. The $K_{1\mathrm{c}}$ value can be estimated if the composition of the particle is known or else it can be identified by calibrating the effective K_{1C}^* with the experimental nucleation data. A realistic range for the value of $K_{1\mathrm{c}}$ for

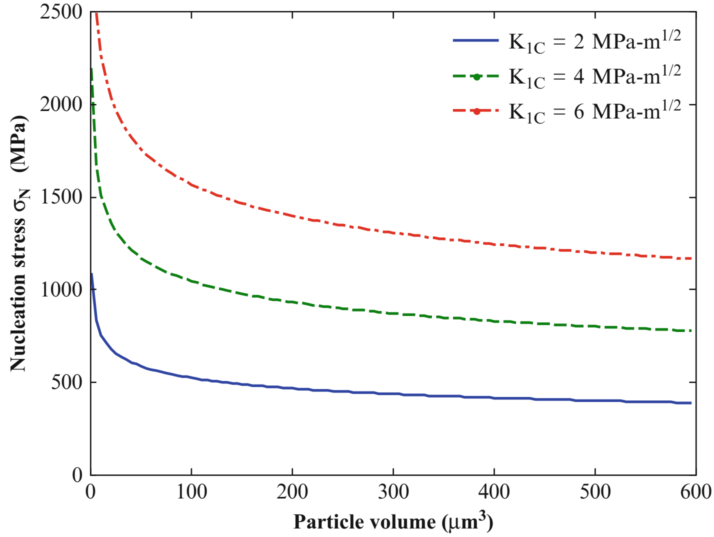

Fig. 9.9 Variation of the nucleation stress with particle size and toughness

brittle materials is 1–10 MPa $\cdot$ m$^{1/2}$ (Moulin et al.). The geometry factor, α, does not have to be determined and can be lumped into the K^*_{1C} value.

The variation of the particle nucleation stress with the volume is presented in Fig. 9.9. The criterion captures the particle size-effect where small particles nucleate at high strains while large particles nucleate at low stresses and are roughly independent of the particle size. The nucleation model also predicts that brittle phases are more likely to crack than more ductile phases. It should be emphasized that the nucleation stress is deeply coupled with the particle size, shape, composition, fracture toughness and the applied stress state as

$$\sigma_N = \sigma_N\left(f_p, W_p, G_p, \kappa_p, \Sigma_{ij}, K^p_{1c}\right) \tag{9.25}$$

and that successful prediction of nucleation relies upon the interrelationships among variables.

The principal contribution of this nucleation treatment is that it is physically realistic and does not contain any calibration parameters. The percolation model is now completely deterministic where fracture is a natural consequence of void nucleation and evolution and no adjustable parameters are employed. The particle distribution, stress state and material properties are solely responsible for the fracture process. All parameters are intrinsic material properties that can be quantified or estimated such as the K_{1c} value.

9.14 Determination of the Initial Dimensions for a Nucleated Void

A three-dimensional ellipsoidal inclusion with semi-axes (a, b, c) and orientation vectors ($\boldsymbol{n_1}$, $\boldsymbol{n_2}$, $\boldsymbol{n_3}$) is embedded within a ductile matrix as shown in Fig. 9.10. The matrix and inclusion are subjected to an external loading that gives rise to a maximum principal stress, Σ_1, along the direction, $\boldsymbol{u}$. The loading is severe enough to induce the particle to fracture or debond from the matrix to form a void. It is assumed that the particle cracks through its center in the direction transverse to the principal loading direction. The dimensions and orientation of the void in this plane are obtained by sectioning the inclusion to form an ellipse on the $\boldsymbol{p}$-$\boldsymbol{n}$ plane where the vectors $\boldsymbol{p}$ and $\boldsymbol{n}$ correspond to the semi-axes of the ellipse denoted a_s and b_s. The void height, c_W, is determined from the assumed aspect ratio for the void at nucleation, W_N. For penny-shaped voids, any value for $W_N < 0.01$ can accurately represent the void. The height of the void can then be calculated as

$$c_W = W_N R_{\mathrm{axi}} = W_N \sqrt{a_s b_s} \tag{9.26}$$

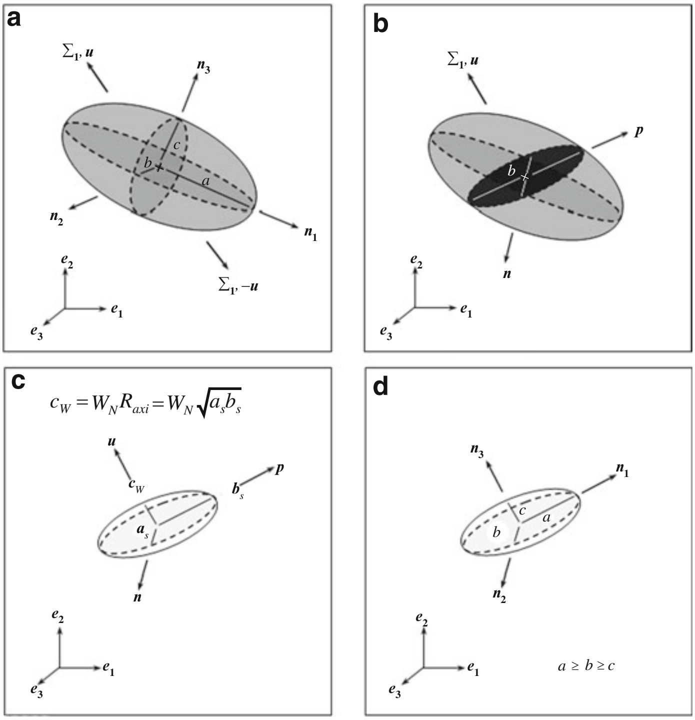

Fig. 9.10 Procedure for modeling void nucleation. (**a**) Ellipsoidal inclusion in a ductile matrix, (**b**) cross-sectional area of the nucleated void, (**c**) penny-shaped void geometry, and (**d**) ordered void geometry and orientation

Finally, the void semi-axes, (c_W,a_s,b_s), and their respective directions, ($\boldsymbol{u}$, $\boldsymbol{p}$, $\boldsymbol{n}$), are ordered so that the semi-axes are now defined as (a, b, c) with directions ($\boldsymbol{n_1}$, $\boldsymbol{n_2}$, $\boldsymbol{n_3}$) and $a \geq b \geq c$. The inclusion that nucleated the void is then removed from further analysis as it is assumed that the particle can only crack once, has a negligible ability to reinforce the material (true for particle cracking) and that any pieces of the broken particle do not significantly impact the subsequent growth of the void (Lassance et al. 2006).

When the principal stresses are comparable as in equal-biaxial tension, the particle may crack transverse to either direction. In this case, the cracking direction is selected as the direction that has the largest particle aspect ratio because prolate particles are more prone to cracking than oblate particles.

9.15 Summary

An approximate integration scheme has been presented to implement a secant-based homogenization theory for particlere inforced plasticity into an existing damage-based constitutive model for ductile fracture. The resulting model can account for the influence of the second-phase particles on void growth, shape evolution, coalescence and material softening. The stress state within particles can also be determined as a function of the particle content, shape and elastic properties. Additionally, the stress state within the matrix material can be estimated with no prior knowledge of its hardening profile. The results for the local stress states will be used to predict void nucleation through particle particle fracture and decohesion in the percolation modelling of ductile fracture in actual particle fields. The present model is best suited for application to sheet metal forming of damage-sensitive industrial alloys where the loading is proportional and the volume fraction of the second-phase particles is low, which is true for most metal forming processes.