Thermal residual stresses in SiC particle reinforced aluminium composites: a study by the Taylor-based nonlocal theory of plasticity

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Abstract. Strain gradient theories have been considered to be an effective means for capturing the size effects on ceramic particle-reinforced metal-matrix composites (MMCp), but the results predicted by them are significantly lower than the corresponding experimental data. One reason might be, that the thermal residual stresses caused by thermal contraction mismatch between the metal matrix and the ceramic particle were neglected in the numerical models. By incorporating the Taylor-based nonlocal theory (TNT) of plasticity, the finite element method (FEM) is applied in the present research, to investigate the effect of thermal residual stresses on the yield stress and average axial stresses of the aluminium matrix reinforced by silicon carbide particles (SiCp/Al). The elements of the matrix have been implemented in the ABAQUS finite element code through its USER-ELEMENT (UEL) interface for TNT plasticity. Some comparisons with the associated literature demonstrate that the numerical model with the thermal residual stresses is more in agreement with the experimental results.

1. Introduction

Ceramic particle-reinforced metal-matrix composites (MMCp) display strong size effect when the characteristic length scale associated with non-uniform plastic deformation is on the order of microns. The most famous case which has described these multiple-scale characteristics of MMCp, is the Lloyds experiment[1] in 1994. He investigated the particle size effect for A356 aluminum alloy reinforced by 15 vol.% SiC particles with two different particle sizes, either 7.5 or 16μm diameter particles. The research showed that small silicon carbide particles with 7.5μm diameter gave significantly higher plastic work hardening than large particles with 16μm diameter.

Various continuum micromechanics methods, such as the modified shear-lag theory[2], Eshelby equivalent inclusion methods[3] and finite element method (FEM)[4-6], failed to predict the influence of particle size on the overall deformation behavior for MMCp, since all the classical plasticity theories do not inherently include an intrinsic length scale[7]. In the past several decades, some plastic

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strain gradient theories have been considered to be an effective means for capturing the size effects in numerical computations, such as phenomenological theories[8, 9], MSG[7] (mechanism-based strain gradient plasticity theory), TNT[10, 11] (Taylor-based nonlocal theory of plasticity), and so on. Strain gradient plasticity theory postulates that the stress at a given point depends not only on the current values and possibly also the previous history of deformation and temperature, but also the neighbourhood of that point. Quite dissimilar to the phenomenological strain gradient plasticity theories[8, 9], TNT and MSG plasticity have clear physical mechanism, which can be applied to void growth, cavitation instabilities and particle-reinforced composites.

Xue et.al[12] used MSG plasticity to investigate the particle size effect and found good agreements with the experiments of aluminum matrix reinforced by silicon carbide particles (SiCp/Al). However, the stress–strain curves predicted by MSG plasticity are still lower than those reported in Lloyd’s experiments[1]. That may be because they have not accounted for other influencing factors in their numerical model such as the effect of thermal residual stress, etc. In addition, Gao and Huang[10] also used TNT plasticity to model the size dependence of MMCp by constructing a spherically symmetric model, which was simplistic and several approximations were made in order to obtain an analytical solution. Yan et al.[6] modified the constitutive relation of metal, with introducing Gao’s analytical solution of TNT to describe the flow behavior of the composite matrix. However, all their work did not take into account the effect of residual stresses, which were caused by differences in the coefficient of thermal expansion between the matrix and the ceramic particles.

In the study, by incorporating the TNT plasticity, FEM is used to investigate the effect of thermal residual stresses on the mechanical behavior of the SiCp/Al composites under the quasi-static uniaxial compressive loads. The elements of the matrix have been implemented in the ABAQUS finite element code through its USER-ELEMENT (UEL) interface for TNT plasticity. In the simulation, the average axial stress of composite matrix follows Taylor hardening law and the strain gradient at each Gaussian point can be obtained in a form of nonlocal integral. The numerical results will be compared with Lloyd’s experiment results[1].

2. Numerical model

2.1. TNT plasticity

TNT plasticity is based on a multi-scale framework linking the microscale notion of statistically stored and geometrically necessary dislocations(GNDs) to the mesoscale notion of plastic strain and strain gradient. The constitutive equations contain neither higher-order stresses nor strain gradients. As a nonlocal integral of strains, strain gradients are introduced in the form of nonlocal variables. The basic principles in the nonlocal constitutive framework can be written as follows: (1) The flow stress obeys the Taylor hardening relations; (2) The GND density is calculated as nonlocal variables expressed in terms of a weighted average of plastic strain; (3) The essential structure of classical plasticity is preserved. In TNT plasticity, the flow stress $\sigma_{\text{flow}}$ is obtained from the Taylor dislocation model as in equation (1).

$$\sigma_{\text{flow}} = M \alpha \mu b \sqrt{\rho} = M \alpha \mu b \sqrt{\rho_0 + \rho_3} = \sigma_{\text{ref}} \sqrt{J^2(\varepsilon)} + \eta l$$

(1)

Where $\rho$ is the total dislocation density, $\rho_3$ is the statistically stored dislocation (SSD) density which accumulates by trapping each other in a random way, $\rho_0$ is the GND density, which is required for compatible deformation of various parts of the non-uniformly deformed material, $M$ is the Taylor factor which acts as an isotropic interpretation of the crystal line anisotropy at the continuum level, $\alpha$ is an empirical material constant in the Taylor dislocation model ranging between 0.1 and 0.5, $\mu$ is the shear modulus, $b$ is the magnitude of Burgers vector, $\sigma_{\text{ref}}$ is a reference stress in uniaxial tension, the function $J(\varepsilon)$ is the non-dimensional function determined from the uniaxial stress-strain curve, $\eta$ is the effective strain gradient, and $l$ is identified as the intrinsic material length introduced by Fleck and Hutchinson[8] as in equation (2).

$$l = 18 \alpha^2 (\mu / \sigma_{\text{ref}})^2 b$$

(2)
In equation (1), the effective strain gradient \( \eta \) is obtained from the deviatoric strain gradient tensor \( \eta'_{ijk} \) by
\[
\eta = \sqrt{\frac{\eta'_{ijk} \eta'_{ijk}}{4}} \tag{3}
\]
where
\[
\eta'_{ijk} = e_{i,j,k} + e_{j,k,i} - e_{k,i,j} - \frac{1}{4} (\delta_{ij} e_{pp,j} + \delta_{jk} e_{pp,i}) \tag{4}
\]

The gradient term, \( e_{ij,k} \) in equation (4) is calculated as nonlocal variables expressed in terms of the weighted average of strains. An eight-node isoparameter element, has been used to evaluate strain, strain gradient and stress. There are two different levels of Gaussian integration in the finite element analysis for TNT plasticity. One is at the element level, which is the same as the classical plasticity theory. Another is at the mesoscale cell level, which is special for the TNT plasticity. There is a square (for a two-dimensional problem) mesoscale cell surrounding each element-level Gaussian integration point. The stresses and effective strain gradients of each element-level Gaussian integration point can be expressed in terms of the nodal displacements via Gaussian integration in the mesoscale cell.

In the numerical model, it is considered that \( \alpha \) is equal to 0.5 and \( l \) is equal to 3.028 \( \mu m \).

2.2. Unite cell model

\[\sigma\]
\[\sigma\]

**Figure 1.** A schematic diagram of the unit cell model for a finite metallic matrix containing a single ceramic particle.

\[\sigma\]
\[\sigma\]

**Figure 2.** A finite element model with the particle diameter \( d \) of 7.5\( \mu m \) and volume fraction of 15%.

A two-dimensional axial symmetry unite cell model[13] was used to investigate the effect of thermal residual stresses on the mechanical characteristics in SiCp/Al composites. Figure 1 is a schematic diagram of the unit cell model for a finite metallic matrix containing a single spherical ceramic particle. Figure 2 is a finite element model with the particle diameter \( d \) of 7.5\( \mu m \) and the particles’ volume fraction of 15%.

The elements of the matrix have been implemented in the ABAQUS finite element code through its UEL interface for TNT plasticity. These elements, which are similar to the conventional eight-node isoparametric elements, also have eight nodes and nine Gauss integration points. The bonding between the particles and the matrix is assumed to be perfect in the analysis.

2.3 Thermal residual stress and material parameters

The thermal contraction mismatch between the reinforcement and the matrix results in a residual stress state, when the composite is cooled from the processing temperature to room temperature. The processing causing thermal residual stresses are simulated by cooling the model composite from the solutionizing temperature of 500°C, where the composite is assumed to be free of internal stresses, to room temperature 20°C, at a constant cooling rate of 10°C·s\(^{-1}\). The thermal deformations only generate linear strains, while the shear strains are zero. The linear strain by thermal expansion is \( \alpha \cdot \Delta T \) at
arbitrary integration point, when the temperature variation is $\Delta T$, where $\alpha$ is the thermal expansion coefficient (CTE).

In the axisymmetric model, the thermal strain caused by the temperature variation in the form of tensor can be written as:

$$\varepsilon_{ij}^0 = \alpha \Delta T \delta_{ij}$$  \hspace{1cm} (5)

In the classical thermal elastic-plastic method, the consistency condition is used to derive a point-wise relation between the stress rate and strain rate,

$$\dot{\sigma} = D^{el}(\sigma) : \dot{\varepsilon}$$  \hspace{1cm} (6)

where $\varepsilon_{ij} = \varepsilon_{ij} - \varepsilon_{ij}^0$, and $D^{el}(\sigma)$ is the local elastic-plastic stiffness tensor. In contrast, the TNT flow theory has a nonlocal relation between the stress rate and strain rate,

$$\dot{\sigma} = G(\epsilon, \dot{\epsilon}, \{\epsilon\}, \{\dot{\epsilon}\})$$  \hspace{1cm} (7)

where $\{\cdots\}$ denotes integral average over a small representative volume.

The flow stress accounting for the effect of GNDs and thermal residual stresses can be given as

$$\sigma_{flow} = \sigma_{ref} \sqrt{f^2(\epsilon) + l\eta}$$  \hspace{1cm} (8)

where the effective strain gradient $\eta$ is described as the equation (3). The effective strain $\epsilon$ in equation (8) is determined in terms of the deviatoric tensor of strain $\epsilon' = (\epsilon_{ij} - \epsilon_{0ij})$ as

$$\epsilon = \sqrt{\frac{1}{2} \epsilon_{ij} \epsilon_{ij}'}$$  \hspace{1cm} (9)

The effective strain gradient $\eta$, which is dissimilar to TNT plasticity without thermal residual stresses, is also the function of $\epsilon'$.

The yield stress of Al matrix dependent of temperature is defined by the experimental result of LEVY[14]. The modulus of elasticity, which is also dependent of temperature, refers to the experimental data of Lloyd[1].

The SiC particle is assumed to be linearly elastic and isotropic. The matrix at room temperature is characterized by using a piecewise elastic-power law hardening relation, to model the uniaxial stress–strain behavior for unreinforced Al alloy. Their material parameters are shown in table 1.

| Material     | Young’s modulus (GPa) | Poisson’s ratio | Initial yield stress (MPa) | Power exponent | CTE ($10^{-6}$·K$^{-1}$) |
|--------------|------------------------|----------------|---------------------------|----------------|---------------------------|
| SiC          | 427                    | 0.17           | -                         | -              | 4                         |
| Al alloy     | 76                     | 0.33           | 208                       | 0.136          | 24                        |

3. Result and discussion

3.1 Effects of thermal residual stresses on average axial stresses

The stress–strain curves without thermal residual stresses, predicted by TNT plasticity and classical elastic-plastic theory and Lloyd’s experimental data[1], are shown in figure 3. The average axial strain in the cell is evaluated by the ratio of the uniform displacement on the top surface dividing the half-cell height. The average axial stress in the cell is determined by the total axial force multiplying the cell cross section area, where the total axial force is obtained from the nodal force of all nodes on the top surface.

The average axial stress predicted by the classical elastic-plastic theory without thermal residual stresses is lower than that predicted by TNT theory, since the classical elastic-plastic theory does not take into account the strain gradient caused by GNDs. But the flow stress predicted by TNT theory is still below Lloyd’s experimental data [1]. Compared with MSG theory, the stress–strain curve without thermal residual stresses predicted by TNT theory for particle diameter size of 7.5μm quantitatively agrees with that done by Xue[12]. It means that some other factors, which were not taken into account
in our current model, influence the predicted results. In fact, there are many factors which may lead to the deviation from the experimental data, such as thermal residual stresses, particle shape, and particle distribution, etc. In this section, we will discuss the effect of thermal residual stresses on the average axial stress of SiCp/Al composites.

\[\text{Figure 3.} \ \text{The stress–strain curves without thermal residual stresses predicted by TNT plasticity and classical elastic-plastic theory and Lloyd’s experimental data.}\]

\[\text{Figure 4.} \ \text{Comparisons of compressive stress-strain curves with and without thermal residual stresses (including Lloyd’s experimental data and the curve predicted by classical theory).}\]

Figure 4 shows comparisons of compressive stress-strain curves with and without thermal residual stresses (including Lloyd’s experimental data and the curve predicted by classical theory). The curve with the existence of thermal residual stresses, shows lower slopes at the early stage of deformation, due to the lower apparent moduli (arising from prior plastic deformation). It explains that the presence of residual stresses enhances the initial strain hardening. The curve then crosses the corresponding curve without thermal residual stresses, and results in higher values of the average axial stress thereafter. The differences in average axial stresses beyond the crossover point persist throughout the
plastic deformation stage. Compared with Lloyd’s experimental data[1], a deviation from the experimental data still exists, but the amplitude of average axial stress is closer to the experimental curve. Both strain hardening and strain gradient due to the thermal residual stresses may lead to the additional plastic hardening. But we think that the strain hardening, rather than strain gradient, provides a major contribution. The effects of strain hardening caused by thermal stresses[14, 15] have been investigated in the past decades, thus we will discuss effects on thermal residual stresses of the effective strain gradient in next section.

3.2 Effects of thermal residual stresses on equivalent strain gradient

For deeper insight into the effects of thermal residual stresses of the equivalent strain gradient during subsequent mechanical loading, the average equivalent strain gradient with and without thermal residual stresses are compared, as shown in figure 5. The average equivalent strain gradient $\eta_{av}$ in the compressive direction of the composite are calculated by using an area average approach as follows,

$$\eta_{av} = \frac{1}{S} \int_{S} \eta dS = \frac{1}{S} \sum_{j=1}^{m} \left( \sum_{i=1}^{n} \eta_{i} |J| J_{i} \right) (n = 1, 2 \cdots 9)$$

where $\eta_{av}$ is the average equivalent strain gradient, $S$ is the total area, $n$ is the total number of Gauss integral points of each element, $m$ is the total number of elements, $\eta_{i}$ is the equivalent strain gradient at the Gauss integral point, and $H_{i}$ and $J_{i}$ are the Gaussian integral weight coefficient and Jacobian determinant at the integral point, respectively.

**Figure 5.** Comparison of the average equivalent strain gradient with and without thermal residual stresses

We can find that the curve with the existence of thermal residual stresses has a nonzero value at the onset of subsequent mechanical loading after cooling. The curve with the existence of thermal residual stresses shows a higher level of $\eta_{av}$, and then crosses the corresponding curve without thermal residual stresses at average axial strain of 0.01. This means that overall yielding takes place at a higher average axial stress value. After the axial strain of 0.01, $\eta_{av}$ without the existence of thermal residual stresses is slightly greater than that with the existence of thermal residual stresses. This reveals that thermal residual stresses have been redistributed and prior strain by thermal residual stresses offsets
the subsequent increase of $\eta_{av}$ to a certain extent. In a word, the thermal residual stresses improve the overall initial yield stress of composites, but offer a less accumulation of strain gradient beyond the crossover point.

The contours of $\eta_{av}$ predicted by TNT plasticity with and without thermal residual stresses at the average axial strain of 0.02 are shown in figure 6. It can be seen that both distribution characteristics are similar, except that the area of high strain gradient region is slightly greater for the case without the thermal residual stresses. This contour also confirms the conclusion of figure 5.

![Figure 6](image)

**Figure 6.** The contour of average equivalent strain gradient predicted by TNT plasticity at the average axial strain of 0.02: (a) without thermal residual stresses; (b) with thermal residual stresses.

4. Summary
In this investigation, a two-dimensional axial symmetry model based on the TNT plasticity is applied to investigate the effects of thermal residual stresses on the strain gradient in SiC particle reinforced aluminium composites. We have obtained the following conclusions:

1. The numerical model with the thermal residual stresses is more in agreement with the experimental results and the prior thermal residual stresses can improve the initial yield stress and flow stress of SiCp/Al composites.
2. The strengthening caused by thermal residual stresses mainly attributes to strain hardening of metal-matrix, not to strain gradient.
3. The contours of the average strain gradient with and without thermal residual stresses have similar distribution characteristics, except that the area of high strain gradient region of the matrix is slightly higher for the case without the thermal residual stresses.

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