Numerical simulation of the influence of particle clustering on tensile behavior of particle reinforced composites; Study of shape of the particles

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Abstract

This paper aims to investigate the influence of particle clustering on the tensile behavior of particle-reinforced composites composed of aluminum matrix and ceramic particles. Matrix was allowed to deform plastically, yet particles had only elastic deformation in a damage free process. By assuming a periodic microstructure, finite element simulations of a unit cell were carried out. The unit cells were modeled with different cluster densities as well as different particle aspect ratios. All particles were assumed to be oblate ellipsoids which were arranged linearly along the loading direction. Uniaxial stress-strain curves were gained through imposing gradual incremental displacements on the surface of the unit cell to the overall far-field strain of four percent. It was shown that clustering increases the plastic strain within ligaments between particles and promotes the strain hardening in the clustered region. Eventually, it causes a considerable increase in the level of the maximum principal stress in particles. The differences in stress-strain behavior among various composite models in macroscopic level were negligible.

Keywords: Particle-reinforced composites, Clustering, Finite Element Method (FEM)

1. Introduction

Dual-phase alloys and particle-reinforced composites are widely used in numerous areas such as automotive and aerospace industries. Dispersed particles improve mechanical properties of the matrix and lead to high strength composites. Several modelling methods have been proposed recently in order to predict mechanical behaviors of these composites. These modelling techniques can be split into two categories: analytical and finite elements methods. In general, analytical methods rely upon the equivalent inclusion method of Eshelby [1] and on their mean-field extensions [2]. There are a number of analytical modelling approaches proposed, such as the tangent-based [3] and secant-based [4] homogenization approaches, which have been relatively successful in terms of predicting non-linear behavior of composite materials. However, in terms of micro-structural details such as stress state within the particles, analytical approaches are not sufficiently accurate [5], because their formulations are based on different simplifying assumptions such as a homogeneous distribution of particles in the matrix [6]. Unlike the analytical approaches, FE techniques enable us to distinguish the influence of heterogeneous particle distribution, which is much more realistic than homogeneous particle distribution [7].

In the study conducted by Abedini et al. [8], the influence of particle clustering on mechanical behavior of particle-reinforced composites has been investigated quantitatively by using the method introduced by Thomson et al. [9] for multi-particle unit cells. Composite material is assumed to be composed of repeated multi-particle unit cells containing spherical particles. Morphology of different types of particle clustering has been investigated so that useful comparisons between different cluster severities and geometries can be made. This method has provided a good understanding of local stress state within particles in a cluster. Local stresses
within clusters have a significant role for the initiation of microvoids which can result in the earlier onset of damage. By taking advantage of the periodic symmetry, the particle field has been reduced to a single unit cell. Based upon FE analysis, Abedini et al. [8] has concluded that as the degree of clustering increases, the flow stress of the composite exhibits a slight increase. The objective of the present article is to perform a quantitative analysis of linear cluster arrangement within unit cell in uniaxial tension. According to Abedini et al.’s work [8], linear cluster morphology was highlighted among other morphologies as the most sensitive cluster type to various stress conditions. Unlike Abedini et al. [8], in the present study, ellipsoidal particles are modeled instead of spherical ones since based on Chawla and Chawla’s [6] results, ellipsoidal particles simulate more realistic geometry comparing to spherical particles.

2. Model Description

2.1. Cluster Geometry

Due to the high sensitivity it indicates [8], linear cluster morphology has been considered. Figure 1 shows one-eighth of a single particle unit cell along with a linear particle arrangement in the cluster. Ellipsoidal particles aligned with loading axis were modeled in clusters with a variety of densities. Here in Figure 1 particles are not depicted in their spots, for the morphology is clearer in this way. Due to the symmetry, only one eighth of each unit cell has been modeled. Each unit cell of the cluster model contains three ellipsoidal particles within it.

![Image of particle unit cell and linear cluster arrangement](image)

Figure 1- One eighth of unit cell for: (a) Single particle, (b) Linear cluster.

As displayed in Eq. 1, severity of a cluster is quantified through the variable $K$ which is equal to the inter cluster spacing, $D$, relative to the inter particle spacing, $d$. The larger the value of $K$, the denser particle clustering is achieved.

$$K = \frac{D}{d}$$  \hspace{1cm} (1)
Cluster densities of $K = 18, 10, 6$ and $3$ were investigated along with aspect ratios of $AR=2,3$ for ellipsoids. The aspect ratio of the unit cell $\frac{L_1}{L_2}$ was assumed to be equal to the aspect ratio of the particles.

![Diagram of unit cell](image)

Figure 2 – One eighth of a unit cell along with symbol definitions, $AR = \frac{a}{b}$.

### 2.2. Boundary Conditions and Material Properties

In order to ensure that the periodic microstructure assumption is still valid, all of the planes of the unit cell are considered to remain planar and to maintain their initial orientation. Displacements along normal directions as well as rotations around all axes are restricted for all three planes of symmetry (planes A, B and C in Figure 1). Uniaxial tension was gained through imposing gradual incremental displacements on the side surface along the $z$ axis to the overall strain of four percent. The small level of overall strain was chosen to support the assumption of damage free composite.

Three-dimensional FE models of particle-reinforced composite were simulated in order to predict the overall uniaxial tensile stress-strain response, local stress fields and local strain fields. Commercial FE software, ABAQUS, was used to perform the simulation. A typical FE mesh with eight-node linear brick elements was used, as is depicted in Figure 3. Each series of meshing was checked for mesh sensitivity, and distortion, which was pointed out through the ABAQUS mesh verification tool, which was found adequately negligible with a sufficiently refined mesh. All simulated particle-reinforced composites were composed of an aluminum matrix and ceramic particles.

It was assumed that the elastic-plastic matrix obeys the hardening rule represented in Eq. 2:

$$\sigma = \sigma_y + K\varepsilon_p^n$$

Where $\varepsilon_p$ and $\sigma_y$ are the accumulated plastic strain and the initial yield stress, respectively and the values of constants, $K$ and $n$, are shown in Table 1 along with other mechanical properties of the constituents.

The bonding between the matrix and particles was assumed to be perfect, and thermal residual stresses were not taken into account. Furthermore, the nucleation of voids by particle cracking or
interface separation was also not considered as the objective of this study is to investigate the influence of particle clustering on the material response before the onset of damage.

![Figure 3- A typical FE mesh for the linear cluster model with AR=2 and K=3.](image)

### Table 1 – Material properties of each of the phases.

<table>
<thead>
<tr>
<th>Material</th>
<th>$E$ (GPa)</th>
<th>Poisson’s ratio</th>
<th>$\sigma_y$ (MPa)</th>
<th>$K$ (MPa)</th>
<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>75</td>
<td>0.3</td>
<td>75</td>
<td>416</td>
<td>0.39</td>
</tr>
<tr>
<td>Ceramic</td>
<td>400</td>
<td>0.2</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

### 3. Results and Discussion

#### 3.1. Macroscopic Response

Overall mechanical behavior of the unit cells under uniaxial tension is reported in this section. Linear clusters containing ellipsoidal particles with different aspect ratios and levels of cluster densities have been studied and compared over the particle volume fraction of 0.01. These results are based on volumetrically averaged, macro stress values with respect to macro strain. Figures 5 and 6 indicate that as $K$ increases (i.e., the cluster becomes denser), the flow stress in the unit cell increases slightly. However, these graphs represent almost the same behaviors in the elastic regime. Moreover, the difference between the largest and the smallest flow stress is so small (around 0.6%) that makes the effect of particle clustering on overall behavior of the unit cells negligible. Therefore, it is concluded that the higher particle clustering increases the work hardening to a very limited degree in the macroscopic scale. All FE results are in qualitative agreement with the results obtained by Abedini et al. [8] for spherical particles.

Another comparison also has been made to analyze clusters with the same clustering density but different particle aspect ratios. According to the definition of aspect ratio presented in Figure 2, spherical particles acquire $AR=1$. This comparison illustrates the influence of particle aspect ratio on the overall response of the composite. The results for ellipsoidal particles (with $AR=2$ and 3) are compared to the corresponding curves for spherical particles ($AR=1$) reproduced from Abedini et al [8]. Figures 7-9 depict overlapping curves of the same cluster density with different aspect ratios of particles. These diagrams show nearly identical curves in the elastic regime and a very limited scatter when plastic deformation becomes dominant. However, in all cases, it is observed that the stress-strain curves with greater particle aspect ratios lie slightly above other curves. It implies that longer oblate ellipsoidal particles make the composite slightly stronger.
Figure 5-Overall behavior of the composite for the ellipsoidal particle linear cluster with $AR=2$ and different values of $K$.

Figure 6-Overall behavior of the composite for the ellipsoidal particle linear cluster with $AR=3$ and different values of $K$. 
Figure 7- Overall behavior of composites for $AR=1,2,3$ with a single inclusion within the cluster.

Figure 8- Overall behavior of composites for $AR=1,2,3$ with a cluster ratio of $K=10$.

Figure 9- Overall behavior of composites for $AR=1,2,3$ with a cluster ratio of $K=18$. 
3.2. Microscopic Response

Although macroscopic response for the composite is important, it does not fully reveal why and how failure occurs in the heterogeneous material. Hence, microscopic response should be investigated since failure begins as a local event. Figures 10 and 11 show the results for volume averaged principal stress in the middle particle of the linear cluster model with respect to far-field strain. Unlike macroscopic responses that were not substantially influenced by cluster densities, Figures 10 and 11 evidently show a significant increase of the principal stress within the particle with increasing the particle clustering density. In other words, the smaller the space between particles, the greater stress is present in the particle. Also, single particle models show the smallest level of stress in comparison with all multi-particle cluster models. As expected, these trends are totally in agreement with the results for spherical particle(s) [8].

After the evaluation of the influence of the cluster density on averaged principal stress in the middle particle, the volumetrically averaged maximum principal stress in the middle particle of the linear cluster model with respect to far-field strain was investigated for models of the same cluster densities (K) and different ARs. Figures 12 and 13 depict the results. Curves representing the behavior of spherical particles (AR=1) are taken from Abedini et al.’s work [8]. According to Figures 12 and 13, as the aspect ratio increases in the composite, the larger maximum principal stress is imposed on the middle particle. Furthermore, the amount of stress experienced by the particle increases as the cluster density increases and this increase is more significant for the cluster models with higher aspect ratio particles.

![Figure 10- Microscopic behavior of middle ellipsoidal particle for linear cluster with AR=2 and different values of K.](image)
The equivalent plastic strain is a direct measure of the level of plastic flow in the matrix. Higher plastic strain in a region causes more hardening, and, consequently, greater stress is transferred into the particles in the region. As Figure 14 indicates, the maximum equivalent plastic strain occurs in the space between particles. Since the maximum plastic strain takes place within clusters, it can be predicted that particle fracture (and consequently damage) is initiated from the clustered area which is in total agreement with experimental results available in the literature [9].
Figure 13- Mechanical behavior of the middle particle in linear cluster model of the composites with $AR=1, 2, 3$ and $K=10$.

Figure 14-Contour plot of the maximum principal plastic strain in the FE model.

4. Conclusions

The traditional analytical and numerical approaches to predict the mechanical behavior of particle-reinforced composites are based on assuming homogeneous distribution of particles within the matrix; however, this assumption is not compatible with real composites. Finite elements simulation of uniaxial tension has been conducted considering particle clusters with different aspect ratios of the particles within the matrix and different densities of clusters. In the work conducted by Abedini et al. [8], linear cluster models were found to be the most sensitive particle clustering arrangement to cluster density variation compared to other cluster geometries. The current study was focused on the effect of linear clusters consisting of ellipsoidal particles on the mechanical behavior of particle-reinforced composites.

In both macro and micro scales, it was evident that increasing the cluster density leads to higher level of average stress experienced by the whole composite and the middle particle. However,
differences in macroscopic stress among different cluster densities were negligible for the same particle volume fraction. Furthermore, influence of particle aspect ratio was evaluated for models with same cluster densities ($K$), in macro and microscopic level. Models with higher aspect ratios demonstrated greater levels of stresses within individual particles, implying that a higher load is being transferred to the particles.

Results obtained from this research indicate that as cluster density increases, so does plastic strain in the ligament and this increase is more significant for the clusters with oblate particles. Therefore, it clearly justifies how an increase in cluster density and particle aspect ratio eventually increases stress both in micro and microscopic scale. All results obtained in this study are in good agreement with experimental and FE results available in the literature.

5. Acknowledgement

The present work was supported by the New Brunswick Innovation Foundation, the AUTO21 Network of Centres of Excellence, and the Natural Sciences and Engineering Research Council of Canada.

6. References


