Shakedown loading capacity prediction of metal-based nanocomposites

Sina Soleimanian¹, Min Chen¹,³, Derrick Tate¹ and Shunqi Zhang²

¹ Department of Industrial Design, Xi’an Jiaotong-Liverpool University, Suzhou
² School of Mechatronic Engineering and Automation, Shanghai University, Shanghai
³ E-mail: Min.Chen@xjtlu.edu.cn

Abstract. Nano reinforcement of metals cannot escape the attention of designers who seek to improve overall performance of engineering structures from automotive components to biomedical devices. Since many engineering structures are susceptible to variable cyclic load, presenting shakedown design of them is of the present research interest. So that, in the present research the shakedown loading capacity of metal based nanocomposite is estimated through finite element discretization and interior point optimization method. Finally, the results are obtained for plate structures subjected to two independent biaxial loads. A maximum improvement of 71.2% is achieved for shakedown load factor of the structure, which means a remarkable improvement in load bearing capacity of the structure.

1. Introduction

Metal-based nanocomposites are widely applied in the automotive, ship, and biomedical industries. The prediction of loading capacities of these materials under unpredictable cyclic loading plays an important role in structural design. As long as the load amplitude exceeds a specific limit higher than the yield strength, the structure may return to the elastic regime following plastic deformations during finite cycles of loading. This return to elastic behavior is referred to as shakedown phenomenon. The sufficient condition for shakedown phenomenon is the presence of residual stresses which can prevent further plastic deformation. In fact, when the structure shakes down, strain values will be bound to a particular elastic range, and the structure deforms safely as a result.

One major condition that needs to be satisfied for the occurrence of the shakedown phenomenon, is that the material should possess an adequate level of ductility to deform plastically. Another requirement is that the load intensity should not exceed the shakedown limit. Otherwise the structure does not shakedown, and it fails due to incremental plasticity, or alternating plasticity (low-cycle fatigue) [1]. There is a wide body of literature on the design of engineering structures under shakedown loads [1-4]. Ure et al. [5] employed linear matching method to evaluate shakedown and ratchet limits of pipe intersections and nozzle-sphere intersections. Simon et al. [6] presented a solution to large-scale shakedown optimization problems by developing of a new algorithm called primal-dual interior point. In this study, the safe design zone of nanocomposite plates based on shakedown criteria is investigated. For this purpose, the shakedown load factor of the structure is optimized through subjecting a system of equalities and inequalities including self-equilibrium condition of the residual stress and failure criteria condition.

Composite materials are usually modelled using multi-scale approaches, like the nano- or micro-scales in material constitution level, or using the meso- or macro-scale in the global structure level.
The link between different scales is the homogenization theory [7]. In this paper, shakedown behaviour of metal-based nanocomposites is studied with smeared material properties. To evaluate the influences of volume fraction of reinforced phase and porosity on shakedown loading capacity, the metal matrix is considered to be magnesium.

2. Design procedure and problem definition

2.1. Definition of shakedown load domain

In the current study, a load domain can be generally expressed in terms of \(n\) loads which could be body forces or surface loads.

\[
P(x, t) = P(\mu_s(t), x) \quad x \in V \text{ or } S_p; \quad s = 1, \ldots, n
\] (1)

Where the parameter \(x\) is any arbitrary position vector of the structure, \(\mu_s\) is the time-dependent parameter reflecting the loading intensity of the \(s^{th}\) load mode. Supposing independence of all loads, the loading domain can be defined as a hyper-parallelepiped in \(r\)-dimensional space of parameters \(\mu_s\):

\[
\mu^-_s \leq \mu_s(t) \leq \mu^+_s \quad s = 1, \ldots, n
\] (2)

Where \(\mu^-_s\) and \(\mu^+_s\) are the lower and upper limits of \(\mu_s\), respectively. In most cases, the variations in the loads are defined as a set of constant applied loads multiplied by a respective load multiplier. Hence, \(P(x, t)\) can be formulated as the following linear form:

\[
P(x, t) = \sum_{s=1}^{n} \mu_s(t) P^0_s(x)
\] (3)

Where \(P^0_s(x)\) is a constant loading regime including number of consecutive independent loads, and \(\mu_s\) denotes the load factor. Therefore, the loading domain \(P\) can be described by a \(n\)-dimensional polyhedron. Figure 1 illustrates a two-dimensional load domain [1, 7].

Figure 1. Two dimensional load domain \(\mathcal{L}\) and \(\alpha \mathcal{L}\), .

The applied load multiplier of \(\mu_s\) can be calculated by equation (4):

\[
\mu_s = [\cos \theta \quad \sin \theta]
\] (4)

Which defines the value of independent applied loads in terms of \(\theta\) angle. As given by equation (3), the magnitude of applied load could be set through a trigonometric relationship using \(\theta\) angle.

2.2. Mathematical formulation of lower bound Shakedown problem

Based on the virtual work principle, equilibrium of stress can be derived as

\[
\int_V \{\varepsilon^*\}^T (a \sigma^* + \vec{\rho}) dV = \int_{\partial V} \{\delta^*\}^T \{p^*\} dS + \int_V \{\delta^*\}^T \{f^*\} dV
\] (5)

Where \(\varepsilon^*\), \(a\), and \(\delta^*\) represent for virtual strain, shakedown load factor, virtual displacement, respectively. Besides, the parameters \(p^*\) and \(f^*\) denote surface and body forces, respectively. According to equation (5), both residual stress \(\vec{\rho}\) and elastic stress \(\sigma^*\) have to be discretized through finite element methods. Considering an isoparametric hexahedral element with \(i=8\) nodes, appropriate nodal shape functions are defined as
Where \( x', y', \) and \( z' \) are the three components of local coordination considered for the element domain denoted by \( x(Ω) \), and \( x_i \) is considered as the nodal global coordination. Mapping from the element domain to the physical domain is possible through the following interpolation:

\[
x(Ω)^e \approx \sum_{i=1}^{N_{NE}} N_i(Ω) x_i^e
\]

(7)

Where NNE represents the number of nodes per element. Similarly, the displacement vector can be mapped from a local field to the global one as given by:

\[
u(Ω)^e \approx \sum_{i=1}^{N_{NE}} N_i(Ω) u_i^e
\]

(8)

The element strain tensor can be obtained by:

\[
\varepsilon = \sum_{i=1}^{N_{NE}} B_i U_i
\]

(10)

Where the \( B_i \) matrix including the derivatives of shape functions with respect to global coordinate components is multiplied by the nodal displacement vector. Consequently, the elastic stress can be discretized as:

\[
\sigma^e = k^{-1} \varepsilon
\]

(11)

Here, the \( K \) matrix is the element elastic stiffness which can be obtained by:

\[
K = \iiint B^T D^{-1} B \, dx \, dy \, dz = \iiint B^T D^{-1} B \, |J| \, dx' \, dy' \, dz'
\]

(12)

Where \( D \) is the fourth-order tensor of elasticity, and the global coordinate components \((x, y, z)\), and \( J \) is the Jacobian matrix which can be defined by:

\[
J = \begin{bmatrix}
\frac{∂x}{∂x'} & \frac{∂y}{∂x'} & \frac{∂z}{∂x'} \\
\frac{∂x}{∂y'} & \frac{∂y}{∂y'} & \frac{∂z}{∂y'} \\
\frac{∂x}{∂z'} & \frac{∂y}{∂z'} & \frac{∂z}{∂z'}
\end{bmatrix}
\]

(13)

Similarly, the residual stress can be discretized as:

\[
\iiint B^T \{\bar{p}\} \, dx \, dy \, dz = \iiint B^T \{\bar{p}\} \, |J| \, dx' \, dy' \, dz'
\]

(14)

To solve the integrations through numerical method, two Gauss points are considered along each axis. Then, the residual stress discretization can be rewritten as:

\[
[C] \{\bar{p}\} = 0
\]

(15)

Where the \( C \) matrix can be given by:

\[
[C] = \sum_{n=1}^{N_{E}} \sum_{m=1}^{N_{GE}} |J| B^T
\]

(16)

\([C]\) stands for the self-equilibrium matrix. Where \( m \), and \( N_{GE} \) is the number of Gauss points per element equals to 8.

Finally, the shakedown optimization problem can be given by equation (17).
In the second constraint, the parameter $P_k$ represents the load vertex, and $S_y$ is the material yield strength. The second constraint corresponds to the failure criterion which is considered according to von Mises equivalent stress here. This generalized convex optimization problem is considered to be solved through interior point optimization algorithm. Finally, the objective of the optimization problem, $\alpha$ (shakedown load factor) could be obtained. As long as complementary angles of $\theta$ are taken, reaching the same stress values and shakedown load factors is a proof of validity for both the FE analysis and optimization steps.

The shakedown load factor could be separated to two coefficients:

$$\begin{array}{c}
\alpha_x \quad \alpha_y
\end{array} = \alpha, \mu_s \quad (18)
$$

The first constraint which corresponds to the self-equilibrium condition of the residual stress field, should be formulated through isoparametric FE discretisation. The second constraint corresponds to the failure criterion which is considered here according to von Mises equivalent stress. The objective function $\alpha$ should be maximized under satisfaction of both equality and inequality conditions for which the structure can safely shakedown [1, 7].

2.3. Large-scale nonlinear optimization solution

There are different mathematical optimization algorithms to solve large scale nonlinear problems. A common optimization solver employed by previous researchers to predict shakedown limit, is IPOPT (interior point optimization) algorithm [8-10]. Besides, the Interior Point Method has proven to be an efficient approach based on our previous study. Furthermore, the modeling language for mathematical programing called AMPL can be used as a software interface to read input data and write it for the optimization algorithm. In the current study the AMPL+ IPOPT solver is adopted to solve the optimization problem numerically.

3. Numerical verification and parametric study

3.1. Verification example

For verification of the present work, as shown in Figure 2(a), an elastic square plate with central hole ($L=100$ mm, $L/D=0.2$, $E=210$ MPa, $\nu=0.3$, $S_y=280$ MPa, $t=2$ mm) subjected to two independent biaxial pressure loads equal to 100 MPa is studied. With the consideration of bi-axis symmetric conditions, the FE model can be simplified as a quarter of the plate, shown in Figure 2(b). The results for shakedown load factor are illustrated in Figure 3. The equal results obtained for complementary angles proves the validity of analysis and optimization methods developed in the current study. The maximum discrepancy of 6.7% between the present results and reference [11] is mainly caused by the different number of elements, further verifying the accuracy of the present approach.

![Figure 2.](image-url)
Figure 3. Comparison of Shakedown load factors with reference [11].

3.2. Parametric study for magnesium based nanocomposites

CNT reinforced magnesium is considered as the nanocomposite material for parametric study. The material properties for the matrix and reinforcement phases are reported in Table 1. The Poisson’s ratio and elastic modulus of nanocomposite are estimated based on the rule of mixtures and the Modified Halpin-Tsai model [12]. Furthermore, the yield strength of nanocomposite for different volume fractions of nanoparticle ($V_f$) and porosity ($p$) are given in in Table 2 [13].

| Material     | Length (nm) | Diameter (nm) | Elastic Modulus (GPa) | Poisson’s Ratio |
|--------------|-------------|---------------|-----------------------|-----------------|
| CNT [13-15]  | 500         | 30            | 1220                  | 0.5             |
| magnesium [16]| -           | -             | 45                    | 0.36            |

Table 2. Yield strength of CNT- magnesium nanocomposite [13].

| $V_f$ | $p=1$ | $p=3$ | $p=5$ |
|-------|-------|-------|-------|
| 0     | 97.6962 | 97.6962 | 97.6962 |
| 0.001 | 133.106 | 126.411 | 119.231 |
| 0.002 | 151.877 | 142.702 | 135.043 |
| 0.003 | 167.235 | 158.161 | 148.718 |

Figure 4. (a) FE model (b) Loading condition and dimensions

The influence of volume fraction and porosity of CNT on shakedown behaviour of a magnesium-based nanocomposite plate ($L=100 \text{ mm}$, $t=5 \text{ mm}$) subjected to two independent pressure loads equal to
200 MPa and simply supported boundary conditions is studied. The FE model is shown in Figure 4 (a). The loading condition and dimensions are given in Figure 4 (b).

4. Results and discussion
First, the mesh convergence is investigated (see Figure 5) considering magnesium plate, and $\Theta=0$. Accordingly, the appropriate number of elements is taken to be 36.

**Figure 5.** Mesh convergence diagram considering pure magnesium, and $\Theta=0$.

Figure 6. The influence of volume fraction of nanoparticle on shakedown load factor of the structure considering constant degree of porosity: (a) $p=1\%$, (b) $p=3\%$, (c) $p=5\%$ for all values of porosity.
Figure 7. The influence of porosity on Shakedown load factor of the structure considering constant volume fraction of nanoparticle: (a) $V_r=0.1\%$, (b) $V_r=0.2\%$, (c) $V_r=0.3\%$.

Figure 6 shows the effect of nanoparticle volume fraction on shakedown load factor. Making a comparison between the diagrams, it can be seen that the variation of shakedown load factor with volume fraction follows the same trend. For the highest degree of porosity ($p=5\%$) and lowest volume fraction of nanoparticle ($V_r=0.1\%$), shakedown load factor of magnesium plate can be refined by 18.1%. While, for the lowest degree of porosity ($p=1\%$) and highest volume fraction of nanoparticle ($V_r=0.3\%$), shakedown load factor of magnesium plate can be refined by 71.2%.

Figure 7 shows the effect of porosity on shakedown load factor. Making a comparison between the diagrams, it can be observed that the variation of shakedown load factor with volume fraction follows the same trend for all values of nanoparticle volume fraction.

5. Conclusions
This work covers the research gap for shakedown design of nanocomposite plates considering homogenized material properties. For thin nanocomposite plates with/without hole subjected to in-plane loading, the present model used an 8-node hexahedral element and interior-point-method optimization algorithm, which leads to reasonable results for prediction of the shakedown load factor. Moreover, the parametric study revealed that, for the nanocomposite with the lowest porosity and highest volume fraction of nanoparticles, the shakedown factor that can be obtained is 71.2% more than the metallic (pure magnesium) structure. To elaborate, the structure possesses higher load-bearing capacity and may shakedown when subjected to a wider range of load amplitudes. Thus, the safety design zone is improved. However, the analytical formulations employed to predict the material
properties cannot be used for heterogeneous materials for which behaviour varies locally. For this reason, determination of material properties based on multiscale approaches is the future research objective of the authors of the present work.

Acknowledgements
The authors thank the funding support NSFC (51805447), Jiangsu Department of Science and Technology (BK20170418), XJTLU Key Program Special Fund (KSF-E-01) and Research Development Fund (RDF-17-02-44).

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