Finite-Element Simulations of Harmonic Structured Materials

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Finite-Element Simulations of Harmonic Structured Materials

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Abstract

Bimodal harmonic structured (HS) materials, is a new class of multi-scale archi-
tected metallic materials having specified topological arrangement of coarse- and ultra-fine grains. HS are experimentally proven to combine both high strength and ductility associated with ultra-fine- and coarse-grained fractions respectively. In this work, finite-element models of HS structured specimens were constructed and their tensile tests were simulated to unravel micro-mechanical mechanisms of plastic deformation.

A constructed 2D-model was successful in capturing expected macroscopic behaviours. It also revealed mechanisms behind superior performance of HS materials compared to their counterparts with bimodal randomly distributed grains.
Preface

This thesis was carried out at the Division of Mechanics, Lund University. I thank Prof. Dmytro Orlov – many were the questions and long were the discussions. I also thank Dr. Aylin Ahadi for her help and support. Fellow student Jakob Salomonsson offered many valuable suggestions.

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1 Introduction

Understanding the mechanical behaviour of a material and constructing material models is fundamental in envisaging its structural applications and for developing new materials. It is also time saving and is often financially advantageous during designing processes.

Recently, a new structure design called Harmonic Structured Materials (HS), was successful in combining the ductility characteristic of coarse-grained materials, and the strength characteristic of their fine-grained counterparts[1]. Through a procedure starting with a mechanical milling of a metal powder, the initially coarse grained powder balls develop a "shell" of fine grains enclosing the coarse grains, or "core". After sintering such powders, the resulting material has a network of fine grains with embedded islands of coarse ones. The refinement of coarse-grained metals have been proven to strengthen materials along with losing most of its ductility. The HS-materials have been more successful in the sense that the enhanced strength does not compromise the ductility.

The research of HS-material has almost exclusively been experimental. Therefore, computational models are necessary for further insights into mechanical performance.

1.1 Objective

The objective of this thesis is to develop a qualitative computational model of HS structure and to simulate tensile tests in software Abaqus/CAE in order to understand the material micro-mechanics and to pave the ground for further development of HS-materials. Analysis will cover deformation up until necking.
2 Theory

2.1 Harmonic structured materials

Typically, metals with average grain-size $> 10\mu m$ have a relatively low yield stress but are very ductile[1]. It has been shown that the refinement of grains in such metals down to sub-micrometer range $d < 1\mu m$, increases the strength of a material at the significant lose in ductility[2]. Using approaches typical for traditional metallurgy, the refined grains become randomly distributed throughout material, without any control over their distribution or architecture. Very fine grains have a limited capacity to store dislocations, and therefore, strain localisation takes place early in the deformation of such materials[3].

In a recent attempt to combine the high strength and high ductility, a new strategy was proposed, and demonstrated success already in early experiments. This strategy involves controlling the amount of refined grains along with their arrangement, and is named "Harmonic structure" (HS). It was found that the properties in HS materials depend not only on the average grain size, but also on their spatial distribution. HS-materials have demonstrated the increase of yield stress for $1.3 - 2.3$ times, while ultimate tensile stress $1.15 - 1.5$ times. At the same time, they either preserved most of their total elongation or increased it[1],[6]. Below follows main steps in the fabrication of HS-materials.

2.1.1 Fabrication of HS-materials

According to [5], main steps in the fabrication of HS-materials are as follows. Consider copper in a fully recrystallised original form with an average grain size of $21 \mu m$, now referred to as "bulk". Now consider same-purity copper in the form of powder. The average particle size is $100 \mu m$, and it has an average grain size of $13 \mu m$. After mechanical milling, the particles develop fine-grained "shell" on their periphery, see schematic picture in Fig. 2.1. These fine grains have an average size of $0.8 \mu m$ and enclose the coarse grains. The volume fraction of fine grains in a powder particle directly depends on the total time of milling, and usually lies between $10 - 40 \%$. 


After milling, the powder is heat treated and rolled multiple times. Final micro structure can be seen in Fig. 2.2[4]. It can be seen as a net of fine grains and regions of coarse grains.

**Figure 2.2:** Topology of shell/core structure in HS copper with fine-grain volume fraction 36%[4]

Fig. 2.3 shows the results of tensile tests on a specimen having such a micro structure. In the graph, this is referred to as MM+HRS (Harmonic). It is compared to the original bulk material cold rolled for a thickness reduction 90%, which has randomly distributed refined grains (average grain size 2.5µm).
As seen in this diagram, the HS-material has higher yield stress than bulk sample along with, higher ultimate tensile stress than CR90, and also elongates more than CR90. These properties are attributed to the micro structure of the HS-material. Note that the Young’s modulus is the same for are the samples. The Young’s modulus is not affected with the change of grain-sizes[7]. On a macro-scale, the sample behaves homogeneously but on a micro-scale it behaves heterogeneously due to difference in the mechanical characteristics of structural components. Fig. 2.4 illustrates the difference in stress-strain behaviour in coarse-grained (CG) and ultra-fine grained materials (UFG) during early deformation stages after a displacement $u$. 

**Figure 2.3:** Stress-strain curves for copper with different micro structures.
The two curves in Fig. 2.4 have the same Young’s modulus but different yields stresses, $\sigma_{YS}^{FG} > \sigma_{YS}^{CG}$. At a displacement $u$, the CG-material is already in a plastic state, while the UFG-material is still elastic. This is the case in the experiment described above. The authors, Orlov et al., have concluded that this leads to the extension of strain hardening stage and therefore strain localisation is delayed. At the stage when plastic flow initiates in the UFG-phase, a decrease in the strain hardening rate takes place, see Fig. 2.4. Necking begins when the strength of the CG-regions equalises to that in the UFG-part, and the capacity of HS material to store lattice defects becomes exhausted. The tensile characteristics of harmonic structured copper presented here are comparable to copper processed by channel angular pressing. This will be used later in an assumption regarding material data.

The results from experiments with HS-material show that the arrangement of refined grains strongly affects mechanical properties. It has also been shown that the ratio of fine/coarse grains has strong effect on achieving a desired strength/ductility ratio[1]. Harmonic structure provides the best tensile performance of a material.

### 2.2 Finite-element formulation for non-linearity

In tensile tests, a specimen is plastically deformed until necking and then fracture. Commercial programs such as Abaqus/CAE, are designed for finite-element simulations and therefore, main steps and details will be presented here for simulations in Abaqus. See [8] and [9] for more information.

Typically, the development of a finite-element formulation begins with the
equations of motion, then introducing a weight function which is approximated by Galerkin’s method. The most convenient way of presenting final formulation is using matrix notations, but during its derivation, index notations may be used. Finally, a full Newton-Raphson solution scheme will be described.

2.2.1 Elasto-plasticity

Assume a material with elasto-plastic behaviour, seen in Fig. 2.5. Up until initial yield stress $\sigma_y$, the material behaves elastically but if higher stresses are reached, $\sigma > \sigma_y$, then plastic strain develops and unloading will result in an irreversible deformation. The total strain at point A is the sum of elastic and plastic strain, i.e.

$$\varepsilon = \varepsilon^e + \varepsilon^p$$

(1)

![Figure 2.5: Typical response of elasto-plastic materials.](image)

A function $f$ is introduced to determine initiation of plasticity. Yield stress changes with plastic loading and therefore, shape, size and position of the yield function $f$ depends also on $n$ internal parameters, $K_\alpha, \alpha = 1, 2, ..., n$.

$$f = f(\sigma_{ij}, K_1, K_2, ..., K_n)$$

(2)

The function describes a surface in the stress space and for values below zero, $f < 0$, the response of such material is elastic. When $f = 0$ plasticity is initialised, and $f > 0$ implies plastic strain development, see Fig. 2.6. The derivation of internal parameters can be found in references given but are not within the focus of this thesis. The stress surface is plotted in the deviatoric plane and the axes are directed along the principal stresses $\sigma_{11}, \sigma_{22}$ and $\sigma_{33}$.
An example of a yield criterion is the von Mises criterion. The stress tensor $\sigma_{ij}$ is a symmetric, second order stress tensor.

$$f(\sigma_{ij}, K) = \sqrt{\frac{1}{2} s_{ij} s_{ji} - \sigma_y - K} \tag{3}$$

where $s_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}$ is the stress deviator tensor and $\delta_{ij}$ is the Kronecker's delta. Fig. 2.6 shows the yield surface for a very first plastic yield development.

In this thesis, tensile test will be simulated and no unloading will occur. For this case, it is sufficient to state that $f = f(\sigma_{ij})$.

### 2.2.2 Stress- and strain tensors

In a Cartesian reference frame, a material point has a vector position $\mathbf{x}_0$ before deformation and $\mathbf{x}$ after deformation. The point has been translated with the vector $\mathbf{u}$. The motion can be expressed as

$$\mathbf{x} = \mathbf{x}_0 + \mathbf{u} \tag{4}$$

The deformation gradient $\mathbf{F}$ is defined as a partial derivative

$$d\mathbf{x} = \begin{bmatrix} \frac{\partial x_1}{\partial x_0^1} & \frac{\partial x_1}{\partial x_0^2} & \frac{\partial x_1}{\partial x_0^3} \\ \frac{\partial x_2}{\partial x_0^1} & \frac{\partial x_2}{\partial x_0^2} & \frac{\partial x_2}{\partial x_0^3} \\ \frac{\partial x_3}{\partial x_0^1} & \frac{\partial x_3}{\partial x_0^2} & \frac{\partial x_3}{\partial x_0^3} \end{bmatrix} d\mathbf{x}_0 = \mathbf{F} d\mathbf{x}_0 \tag{5}$$

and the displacement gradient $\mathbf{D}$ is defined as a partial derivative

$$d\mathbf{x} = \begin{bmatrix} \frac{\partial u_1}{\partial x_0^1} & \frac{\partial u_1}{\partial x_0^2} & \frac{\partial u_1}{\partial x_0^3} \\ \frac{\partial u_2}{\partial x_0^1} & \frac{\partial u_2}{\partial x_0^2} & \frac{\partial u_2}{\partial x_0^3} \\ \frac{\partial u_3}{\partial x_0^1} & \frac{\partial u_3}{\partial x_0^2} & \frac{\partial u_3}{\partial x_0^3} \end{bmatrix} d\mathbf{x}_0 = \mathbf{D} d\mathbf{x}_0 \tag{6}$$

The Green’s strain tensor $\mathbf{E}$ is defined as

$$\mathbf{E} = \frac{1}{2} (\mathbf{D} + \mathbf{D}^T + \mathbf{D}^T \mathbf{D}) \tag{7}$$
and is a symmetric, second order strain tensor. Its corresponding stress tensor $\sigma$ is the second Piola-Kirchhoff stress tensor.

For elastic conditions, it is well known that the relation between stress and strain is described by

$$\sigma_{ij} = D_{ijkl} \varepsilon_{kl}$$

where $D_{ijkl}$ is the elastic stiffness tensor. The constitutive relation for elasto-plastic behaviour between stress and total strain for elasto-plastic material is

$$\dot{\sigma}_{ij} = D_{ijkl}^p \dot{\varepsilon}_{kl}$$

where $D_{ijkl}^p$ is the tangential stiffness equal to the elastic stiffness if elastic loading is present, and is equal to elasto-plastic tangent stiffness if plastic loading is present. This implies that if the increment of strain is known then the increment of stress is also known. See [9] for the derivation of tensor $D_{ijkl}^p$. The tensors $\sigma_{ij}$ and $\varepsilon_{kl}$ above are both second order symmetric tensors when considering isotropic material. This means for example that $\varepsilon_{kl} = \varepsilon_{lk}$. Therefore, the matrix formulation below is possible and convenient. The strains and stresses can assume the form

$$\sigma = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{bmatrix}, \quad \varepsilon = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{13} \\ 2\varepsilon_{23} \end{bmatrix}$$

### 2.2.3 Finite-element formulation

The part of an arbitrary body has volume $V$ and surface $S$. The traction vector $t_i$ acts along boundary surface with outer normal unit vector $n_j$, and a body vector $b_i$ acts in region $V$. The equations of motions, or the strong form, takes the form

$$\frac{\partial \sigma_{ij}}{\partial x_j} + b_i = 0$$

where $\frac{\partial \sigma_{ij}}{\partial x_j} = t_i$ has been used and static conditions have been assumed. By multiplying by an arbitrary weight vector $v_i$, and then integrating over the entire body the following is obtained.

$$\int_V v_i (\frac{\partial \sigma_{ij}}{\partial x_j} + b_i) \, dV = 0$$

By the use of Gauss’s divergence theorem $\int_V div \frac{\partial q_j}{\partial x_j} \, dV = \int_S q_j n_j \, dS$, the weak formulation is finally obtained.

$$\int_V \varepsilon^v_{ij} \sigma_{ij} \, dV = \int_S v_i t_i \, dS + \int_V v_i b_i \, dV$$
where the quantity $\epsilon_{ij}^v$ defined by

$$
\epsilon_{ij}^v = \frac{1}{2} (v_{i,j} + v_{j,i})
$$

is related to the weight vector $v_i$ but has nothing to do with the displacement vector $u_i$, rather it is only related to the weight vector in the same manner as the strain to the displacement. The weak formulation is now expressed in matrix notations where the following is used.

$$
\begin{bmatrix}
\epsilon_{11}^v \\
\epsilon_{22}^v \\
\epsilon_{33}^v \\
\epsilon_{12}^v \\
\epsilon_{13}^v \\
\epsilon_{23}^v
\end{bmatrix}, \quad
\begin{bmatrix}
t_1 \\
t_2 \\
t_3
\end{bmatrix}, \quad
\begin{bmatrix}
b_1 \\
b_2 \\
b_3
\end{bmatrix}, \quad
\begin{bmatrix}
v_1 \\
v_2 \\
v_3
\end{bmatrix}
$$

The weak form of the equations of motions can be written as

$$
\int_V (\epsilon^v)^T \sigma \, dV = \int_S v^T t \, dS + \int_V v^T b \, dV
$$

An important assumption of the finite-element method is that the displacement $u = u(x_i, t)$ can be approximated as

$$
u = Na
$$

where $N = N(x_i)$ contains the global shape functions and $a = a(t)$ includes all the nodal displacements of the body. Similarly, strain and the arbitrary weight function can, with Galerkin’s method, be approximated as

$$
\epsilon = Ba \quad \epsilon^v = Bc
$$

where $B = B(x_i)$ is derived from $N$ and $c$ is arbitrary. After some manipulation, the final formulation is obtained

$$
\int_V B^T \sigma \, dV - \int_S N^T t \, dS - \int_V N^T b \, dV = 0
$$

From this formulation, the internal forces $f_{int}$ and the external forces $f_{ext}$ are recognised as the following vectors

$$
f_{int} = \int_V B^T \sigma \, dV; \quad f_{ext} = \int_S N^T t \, dS + \int_V N^T b \, dV
$$

2.2.4 Solution of equilibrium equations

In the equilibrium equations in (19), the external and internal forces should cancel each other out. In the beginning of a new load increment this is not the
case and there isn’t any estimate of a new displacement. An estimation is made from the residual, \( \Psi \), defined as

\[
\Psi(a) = f_{int}(a) - f_{ext} = 0
\]  

(21)

Because the external forces are not a function of the nodal displacement \( a \), the derivative of the internal forces is

\[
\delta f_{int} = -\delta \Psi = -\frac{df_{int}}{da} \delta a = -K_t \delta a
\]  

(22)

where \( K_t \) is the tangent stiffness matrix. Equation (22) can be rewritten as

\[
\delta a = K_t^{-1} \Psi(a)
\]  

(23)

Now, the nodal displacement vector can be updated according to

\[
a = a + \delta a
\]  

(24)

Using the constitutive relation from (9), equation (20) can identify the derivative \( \partial \Psi / \partial a \) as

\[
K_t = \int_V B^T \frac{d\sigma}{da} \, dV = \int_V B^T D_t B \, dV
\]  

(25)

In a full Newton-Raphson scheme, the iteration starts from a state of equilibrium, \( n \), where displacements, strains and stresses are known. A new load increment creates a residual, a difference between internal forces - represented by a graph in Fig. 2.7 - and external forces.

\[\text{Figure 2.7: Newton-Raphson scheme}\]
At every iteration, a new increment generates a new tangent stiffness matrix, see (23). This is characteristic for a full Newton-Raphson scheme. Nodal displacements are updated according to (24). Then, strains are calculated according to (17) and stresses can be calculated by approximating integrals of strain increments, see [9]. Finally, internal forces vector $f_{int}$ can be calculated and the iteration continues up until state $n + 1$ where the residual reaches a predefined tolerance value.
3 Method

For the visualisation of the behaviour of HS-materials, tensile tests will be simulated in Abaqus/CAE. A specimen having dimensions 1x1x5 mm is to be deformed in tension. Symmetry conditions will be applied. The main idea of the modelling of the microstructure is to have a certain volume fraction of coarse and fine grains and within these two phases, to have a distinct grain size. The two phases will inherit their material behaviour respectively, i.e. the ”cores” will be assigned the elasto-plastic behaviour of a coarse-grained material and the ”shells” will be assigned the elasto-plastic behaviour of a fine-grained material. No boundary condition is specified between the two phases other than the entire model should be considered as a solid with different properties in the phases. Displacement boundary conditions will be applied. As a solution method, a full Newton-Raphson method is chosen. Any residual stresses or deformation that could remain from fabricating HS-material (cf. section 2.1.1) is not taken into account. Isotropy and room temperature are assumed. As a validation of the accuracy of HS-structuring, the structure is simulated for homogeneous coarse- and fine-grained materials.

3.1 Models

A 2D-specimen with harmonic micro-structure, a 3D-specimen with harmonic micro-structure, and a 2D-model with randomly distributed fine grains (UFG-phase) are constructed.

Model 2D-HS. A 2D-model, see Fig. 3.1, in constructed with the fine/coarse ratio $R = 0.4$ where $R$ is defined as

$$R = \frac{\text{Volume}_{\text{shell}}}{\text{Volume}_{\text{total}}}$$

(26)

This volume ratio is within the range of those used in earlier experiments, cf. section 2.1.1, and was optimal in those experiments. The model has the dimensions 0.5x2.5 mm. This model is subjected to the following boundary conditions: the left and upper surface edges are subjected to x- and y-symmetry respectively while the right edge is pulled in x-direction.
Model 3D HS. A 3D-model of HS-structure is created by repeating a unit cell resembling FCC unit cell. The "cores", among themselves adjacent but not in contact, are constructed as half-spherical and quarters of a sphere. When assembled, the model has the solid network of "shell" (fine grains) with embedded islands of "cores" (coarse grains), see Fig. 3.2.

The 3D-model above has symmetry conditions and dimensions 0.5x0.5x2.5 mm. The volume ratio of fine and coarse grains is $R = 0.4$. The following boundary conditions will be applied to the 3D-model: the surface "A" is pulled along x-axis. The surface opposite of surface "B" is assigned z-symmetry, surface "C" is assigned y-symmetry, and finally the opposite surface of surface "A" is assigned x-symmetry.

This kind of FCC-structure in the 3D-case has a lowest limit of volume ratio which is directly connected to milling time, cf section 2.1. This limit is $R_{min} \approx 0.26$. Lower values than this will cause the spheres to overlap. The lowest limit in the 2D-case is $R_{min} \approx 0.21$. To obtain ratios beyond these limits, other structure arrangements should be investigated.

Model 2D-Random. As a comparison to the HS-structure, this model is
created with approximately the same ratio of R but with a random distribution of UFG-phase, see Fig. 3.3. Dimensions of the specimen and boundary conditions are the same as for the 2D HS-model.

![A 2D-model with randomly distributed UFG-phase.](image)

**Figure 3.3:** A 2D-model with randomly distributed UFG-phase.

### 3.2 Material

The material to be used is Nickel. True stress-strain data for the coarse-grained material (CG) comes from an in-house experiment and can be seen in Fig. 3.4. The data is extrapolated up to the strain value of 1.2 (originally reaching strain value 0.4). Due to the lack of data for UFG nickel, the stresses for strain value 1 - 1.2 of the coarse grained data is extracted and used as fine-grained material (UFG). It is possible to reach these strain values with tests other than tensile, see [10]. For the CG-material, Young’s modulus is \( E = 210 \, \text{GPa} \), yield stress \( Y = 185 \, \text{MPa} \), Poisson’s ratio \( v = 0.31 \), taken from [11]. The UFG-material has the yield stress of \( Y = 925 \, \text{MPa} \) and Young’s modulus and Poisson’s ratio is the same as for the CG-material. Both materials are assumed to have a distinct yield stress. Fig. 3.4 shows true stress-strain curves for an arbitrary coarse-grained material (CG) and its ultrafine-grained counterpart (UFG) which will be used in this qualitative model.
Figure 3.4: True stress-strain curves of CG and UFG (Nickel).

3.3 Meshing

The nature of the HS-models demands, unlike many others, local areas of mesh refinement throughout entire specimen, located around the "cores". First simulations have shown these areas as critical. For the 2D-model, this is achieved by introducing artificial lines, assigning an overall coarse meshing, and then specifying a higher node density around curves, in this case the "cores" periphery. For the 3D-model, these artificial lines are inherited automatically from the modelling of unit cells. Triangular (2D) and tetrahedral (3D) elements are used.

Fig. 3.5 shows a mesh of approximately 692,000 elements with refinements around the "cores".

Figure 3.5: Mesh for the 2D HS-model with ≈692k tri-elements.
The 3D-model demands many more elements if this similar refinement is required. A single cube has, with the same mesh settings as in Fig. 3.5, over 1.3 million elements while the entire model having 5*5*25 cubes (tot. > 800 million elements). The tetrahedral element with its 12 degrees of freedom requires a large amount of memory. It could be mentioned that a mesh of ≈15 million elements requires approximately 170 gb in hard drive memory (suggested by Abaqus/CAE). Because of this, a mesh of (only) 5.1 million elements will be used.

Figure 3.6: Left: Mesh of 3D-model to be simulated. Right: Ideal mesh.
4 Results

A table summarising the results of the simulations is shown below. No stress-strain curve was generated for the Random model since no apparent representative volume element was available.

<table>
<thead>
<tr>
<th>Model</th>
<th>Elongation to necking (mm)</th>
<th>Yield stress (MPa)</th>
<th>Ultimate tensile stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full CG</td>
<td>3.0 (extr. pol.)</td>
<td>185</td>
<td>1007 (extrapol.)</td>
</tr>
<tr>
<td>Full UFG</td>
<td>0.50</td>
<td>925</td>
<td>1007</td>
</tr>
<tr>
<td>&quot;Random&quot;</td>
<td>0.10</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2D</td>
<td>0.63</td>
<td>390</td>
<td>733</td>
</tr>
<tr>
<td>3D</td>
<td>1.2</td>
<td>200</td>
<td>400</td>
</tr>
</tbody>
</table>

4.1 Results 2D-models

Plastic flow. Figure 4.1 shows the 2D HS-model after deformation. An elongation of 0.63 mm was possible before the occurrence of strain localisation. The bottom (free) surface has a wave-like pattern repeating itself along cores/shell.

![Figure 4.1: Deformation of 2D HS-model.](image)

Mesh convergence. Fig. 4.2 shows the stress-strain results from four different meshes where convergence was achieved with the mesh of 692,260 elements. Stress- and strain data are averaged from the centre of cross section. A curve representing the "Rule of mixture", for 40% CG and 60% UFG up to strain value 0.2 is also presented on the diagram. The HS-structured model with both fractions assigned, CG- or UFG-properties (homogeneous materials) is also indicated for the model verification. These two results are named "CG-simulated" and "UFG-simulated", respectively. The CG-simulated curve diverges slightly from experimental one at high strain level, but these values are not reached in the HS-model of the CG-phases.

Let's consider the curve "692,260 elements", which shows stress-strain results from the 2D HS-model. It can be seen that the yield stress is at around 350 MPa. This is higher than that of the CG-material (185 MPa). The inflection of the curve starts after stress reaching 185 MPa, because of the beginning of
plastic flow in the "cores". After 350 MPa, an intensive strain hardening takes place until the strain level of 0.21, just until the end of UFG-data availability. Its ultimate tensile strength is 733 MPa, which is higher than the CG-stress and the curve "Rule of mixture" at this strain at the same strain level.

![Stress-strain curves from 2D-simulations, material data and mathematic representation of CG- and UFG contribution.](image)

**Figure 4.2:** Stress-strain curves from 2D-simulations, material data and mathematic representation of CG- and UFG contribution.

**Stress- and strain distribution.** Fig. 4.3 and Fig. 4.4 show a difference in stress and strain gradients, represented by von Mises stress and equivalent plastic strain (PEEQ) distributions just before or at very beginning (in the case of the "random" model) of strain localisation. Strain localisation takes place in the "random" model approximately at displacement $d = 1$ mm and at displacement $d = 0.63$ mm in the HS-model. This can be attributed to the morphology of structure. The ultimate tensile stresses in the "shell" regions has already reached the highest possible values. Fig. 4.4 shows the plastic strain concentrations in the two models. Note several strain localisations in the "Random" model while concentrations in the HS-model do not reach those values and are located repeatedly in "cores" and their periphery.
Figure 4.3: von Mises stress concentrations in 2D ”Random”- (top) and HS-model (bottom).

Figure 4.4: Plastic strain concentrations in 2D ”Random” (top) and HS-model (bottom).

Local stress-strain distribution. Fig. 4.5 shows the magnified view of the lower left corner of the specimen. The von Mises stresses and PEEQ are plotted in the deformed configuration. On the left edge of these pictures, x-symmetry condition was applied while the upper and right edges are cut sections.

The HS-material tolerates a large difference in stresses between the two phases, ”shells” and ”cores” without any strain localisation. The highest stresses of the UFG-material are generally found between two adjacent ”cores”, see Fig. 4.5. The ”cores” are more elliptic after deformation. The highest strains are found in the centre of the ”cores” and symmetrically on their periphery. Another
feature is the general rise of stress- and strain level at subsurface. This is the case for both the UFG- and the CG-areas. The free surface shows a wavy pattern. This can be explained by the absence of material outside contributing to homogeneity of plastic flow, which results to a wavy pattern along the free outer surface.

Figure 4.5: von Mises stress- and plastic strain concentration in 2D HS model - a magnified view.
Stress/strain distribution and evolution. Fig. 4.6 shows bottom left cell of the specimen and its stress-strain evolution in the undeformed configuration. The contour plots show von Mises stress- and plastic strain in columns 1 and 2 respectively. See section 3.2 for material properties and limits.

According to Fig. 2.3, the entire specimen should be in the elastic state until a stress level in the "cores" reaches its yield stress (185 MPa). Pictures a1 and a2 in Fig. 4.6 show higher stresses begin developing in the area between two adjacent cores in the "shell" region. In row a, no plastic flow is reached. From row b, it can be seen that plastic flow develops early in the "cores" while high (elastic) stresses develop in the "shell" region. This trend continues throughout rows b and c and finally, in row d, plastic condition is broadly spread in the shell region except in the region most distant from all "cores" (green region). Row d, column 2 shows that the most critical areas are those red parts at the boundary between "cores" and "shell" where strain localisation should be expected.
Figure 4.6: Stress- (column 1) and corresponding strain (column 2) evolution in the undeformed configuration.
Among many tools, Abaqus/CAE can reveal profiles of stress, strains and other parameter distributions along paths across the specimen.

One profile was created along the left side of the specimen from its top to bottom. The stress- and strain values along this are plotted for further analysis, see Fig. 4.7. Another profile starts from the bottom left corner and follows the surface the distance of five cells, see Fig. 4.8. Both paths are created in the undeformed configuration after displacement 0.63 mm. Fig. 4.7 a shows principal stresses, b shows strain components, and c shows a plot of von Mises stresses and plastic strains. The diameter of a core is approximately 0.6 mm. Peaks and valleys on the plots in Fig. 4.7 correspond to the contour plots in Fig. 4.5. Periodic phases result in curves having a distinct pattern. The "twin peaks" in Fig. 4.7 a are located within the "shell" regions, while the smooth "hills" are stresses across the "cores". Due to the direction of loading conditions (extension in x-direction), the stresses in this direction, S11, are the highest. An apparent response of the material is to elongate in x-direction and contract in y-direction. The profile selected here is along the cross section and it crosses regions of hard- and soft material, each having different responses. The significant periodic variation of stresses and strain in Fig. 4.7 are therefore located at the boundaries of core and shell phases. Note from Fig. 4.7 that the deformation of the specimen in cross section causes a tension/compression in y-direction, plotted as S22. The S22 component is positive in the "shell" regions while negative in the "cores", which explains the wavy pattern of the specimen free surface. Fig. 4.7 b shows strain components and describes the final elliptic shapes of originally perfectly round circles. Component PE11 and PE22 reach their peaks at the centre of the "cores" resulting in an elliptic shape. Let's analyse now Fig. 4.7 c and the left side of the von Mises stress curve. As explained earlier, this path starts at the upper left corner of the specimen and ends at the bottom. The start of the curve corresponds to the "shell" region, and has the value 564 MPa. It then rises and before reaching the boundary of CG-phase, reaches 927 MPa, a stress level just under yield stress (935 MPa). This corresponds well to other curve in the same figure, which shows the plastic strain along the same path (no plastic flow). This shows that along this edge, or any other vertical path that goes through the centre of "cores", no plastic flow is reached in the "shell"-region. This is in good agreement with Fig. 4.5 and 4.6 where the ultimate tensile stresses for the UFG-phase has been reached. Those stresses are located in the shortest distance between two "cores" and are not on these paths. By following the curves in Fig. 4.7 c, it is seen that plasticity is developed in the "core" and stresses over 600 MPa are reached. The pattern then continues until the end of the path where stresses and strains both (plastic) rise above peaks typical in the pattern, which suggests a significant localised (sub-)surface deformation.

The bottom profile, Fig. 4.8 a shows stress components. Component S11 reveals repeating alternation in tension and compression located in the "shell"-region. The S11 component is high and somewhat even across the "cores". In picture b, it is seen that only the "cores" experience plastic strain. Fig. 4.8 c indicates together stresses and plastic strains in the plot to reveal different
responses in shell/cores.

Figure 4.7: Stress/strain data along left surface edge.
Figure 4.8: Stress/strain data along a part of bottom edge.
Strain localisation. So far, the analysis have covered deformation up until strain localisation (0.63 mm translation). By pulling the specimen just over this limit, excessive element deformation takes place. Contour plots of stress- and strain components at the origin of strain localisation are shown below.

In general, the results are in accordance with Fig. 4.7 and Fig. 4.8. Fig. 4.9 and Fig. 4.10 show that normal components in x-direction are the highest followed by those in y-direction and shear xy-direction. Two latter alternate in tension and compression throughout the specimen. It is seen that stress- and strain localisation begins inside the material in the regions located at the shortest distance between two "cores" where component S22 alternates between tension and compression over a very short distance.
Figure 4.9: Stress components and their concentrations.
Figure 4.10: Strain components and their concentrations.
4.2 Results 3D-model

It was possible to deform the 3D-model for 1.2 mm before strain localisation occurred. The topology of the deformed structure resembles that of the 2D HS-model, see Fig. 4.11. A wave pattern along the surfaces could not be observed because of the coarse mesh since the latter does not have sufficient resolution. Further details on stress- and strain components can be found in appendix.

![Deformation of 3D model after tensile test.](image)

**Figure 4.11:** Deformation of 3D model after tensile test.

Fig. 4.12 shows stress-strain curves from the 3D- and 2D-models. Unlike in the 2D-model, the stress-strain data for UFG-phase in this case was assumed constant at the latest (highest) known stress, i.e. higher elongation was possible than in the case of 2D-model. The description of this stress-strain curve is very similar to that in the 2D-case. The only principal difference is that the inflection of stress-strain curve starts at significantly lower stress values, upon the beginning of plastic flow in the CG area. The overall results from the 3D-simulations follow the same pattern, as been seen in the 2D-model. The highest stresses and strains are found in the x-direction. The evolution of stress-strain in shell/cores is also similar. However, the coarse mesh in 3D-model does not result in representative results at sufficient details.
5 Conclusions and future work

Finite-element models of specimens with bimodal harmonic and random structures have been developed. Both 2D- and 3D-models were constructed but sufficiently fine mesh was only possible to generate for the 2D-models due to the constraints in our computational power. The 3D-model required unacceptably large hard drive space, which led to a simulation with unacceptably coarse mesh. Nevertheless, it was found that 2D- and 3D-models are comparable in general. The analysis allowed to explain the superiority of harmonic structure performance. In particular, HS materials capitalise on the strength of hard phase and ductility of soft one. The specific architecture of HS materials allowed to increase yield stress yet allowing an extended strain hardening. The ultimate tensile strength was also increased. Strain localisation begins inside the HS material, on the interface of the phases. This level of strain limited the simulation, but introduction of a "damage" behaviour in our model should allow simulations beyond this level.

For future work, real experimental data or physically justified more complex material models can be used to further improve the accuracy of the model. The introduction of damage model and re-meshing, will also extend accessibility of deformation simulations.
Figure 6.1: Contour plots of stress components of 2D HS-model at highest tensile strain.
Figure 6.2: Contour plots of strain components of 2D HS-model at highest tensile strain.
Figure 6.3: Contour plots of the stress components. Cut has been made in the yz-plane in 3D-model.
Figure 6.4: Contour plots of the strain components. Cut has been made in the yz-plane in 3D-model.
References

[1] Z. Zhang, D. Orlov, SK. Vajpai, K. Ameyama, 2015, 17, No. 6, ADVANCED ENGINEERING MATERIALS.


