CONTINUUM MECHANICAL UNIT CELL MODELS FOR STUDYING THE THERMOMECHANICAL BEHAVIOR OF HIGH SPEED TOOL STEELS

H.J. Böhm, T. Drabek and A. Eckschlager
Christian Doppler Laboratory
for Functionally Oriented Materials Design,
Institute of Lightweight Structures and Aerospace Engineering,
Vienna University of Technology, Vienna, Austria

Abstract The thermomechanical behavior of high speed tool steels is studied by a continuum micromechanical approach. The simulations are based on three-dimensional unit cell models that contain a number of randomly positioned spherical carbides embedded in a thermoelastoplastic steel matrix. Models of this type allow effects of the geometrical arrangement of the primary carbides to be investigated for a wide range of loading conditions. In the present study emphasis is put on modeling the thermal residual stresses caused by the thermal expansion mismatch between matrix and carbides. The predictions indicate that even though such thermal residual stresses can reach considerable magnitudes, their influence on the overall stiffness of tool steels typically is small and their effect on the strength also is minor.

Keywords: continuum micromechanics, unit cell models, thermal residual stress
LIST OF SYMBOLS

$\alpha$  coefficient of thermal expansion  
$E$  Young’s modulus  
$\varepsilon_{eqv,p}$  accumulated equivalent plastic strain  
$\nu$  Poisson number  
$h$  hardening coefficient (Ludwik law)  
$m$  Weibull modulus  
$n$  hardening exponent (Ludwik law)  
$P_i$  fracture probability of $i$-th particle  
$\sigma_1$  maximum principal stress  
$\sigma_{eqv}$  von Mises equivalent stress  
$\sigma_f$  characteristic strength  
$\sigma_m$  mean stress  
$\sigma_y$  flow stress  
$\sigma_{y,0}$  initial yield stress  
$V_0$  reference volume  
$\xi$  carbide volume fraction

INTRODUCTION

Due to their combination of high stiffness and strength with substantial fracture toughness and wear resistance, high speed tool steels (HSSs) are a group of materials of major technological importance. Many aspects of their thermomechanical behavior are not yet fully understood, however, which has stimulated a continuing interest in experimental and theoretical research. HSSs derive their application relevant properties from their heterogeneous structure. At length scales of the order of a few micrometers this takes the form of primary carbides embedded in a martensitic–austenitic steel matrix, which, in turn, contains much smaller secondary carbides.  

The present study concentrates on modeling at the length scale of the primary carbides, where HSSs may be viewed as a special class of particle reinforced ductile matrix composites and can be studied by the methods of continuum micromechanics. The basic idea underlying such approaches is to describe the thermomechanical behavior of inhomogeneous materials on the basis of the material properties and the geometrical arrangements of
their constituents. A typical aim of micromechanical analyses is to study problems that are difficult or impossible to answer by experiments, such as obtaining information on the influence of the geometrical arrangement of the primary carbides on the stiffness and strength properties of tool steels.

The most important approaches in continuum micromechanics are, on the one hand, mean field and variational schemes for analytically or semi-analytically estimating or bounding the thermomechanical responses of inhomogeneous materials and, on the other hand, numerically-based methods that aim at studying specific phase arrangements (“microgeometries”) at a high level of detail. The most important representatives of the latter group of methods are unit cell analyses that use periodic “model composites” for describing materials that are free of damage or show distributed damage, and embedded cell approaches that focus on localized regions of special interest, such as crack tips.

A considerable body of literature on micromechanical studies of ductile matrix composites is available, most of which have been directed at the thermomechanical behavior of aluminum- or titanium-based metal matrix composites (MMCs). A number of publications, however, have been specifically directed at modelling the mechanical behavior of tool steels and related materials: Two-dimensional unit cell models were reported which focus on exploring the initiation of local damage in HSSs by ductile or creep failure of the matrix, by brittle fracture of the particles and/or by interfacial decohesion, see e.g. [1, 2, 3]. Also, a few studies using three-dimensional unit cells have been published [4, 5]. Macroracks in tool steels were described by planar embedded cell models that, on the one hand, used microgeometries obtained from metallographical sections of HSSs [6, 7] and, on the other hand, compared specific generic arrangements of carbides [8]. In addition, hierarchical schemes [5, 9] were used to investigate the thermomechanical behavior of conventionally produced HSSs, in which the carbides tend to be concentrated in clusters or layers.

A number of recent studies have pointed out that considerable errors may be introduced into predictions for the overall responses and especially for the microscale stress and strain distributions when two-dimensional models are used for describing particle reinforced composites [10, 11, 12]. It is also of interest that relatively small volume elements (i.e. unit cells containing a limited number of particles) can give excellent results for the elastic [13] and good results for the inelastic [11] behavior of overall isotropic ma-
materials that contain spherical particulate reinforcements. Accordingly, the most promising micromechanical modelling approach for HSSs appear to be three-dimensional unit cell or embedded cell models in which a number of randomly positioned carbides approximate the phase arrangements of the actual materials.

The major difficulty encountered in micromechanical analyses of HSSs lie in the limited availability of reliable stiffness and strength data for the steel matrix, the carbides and the interface between them. In addition, studies based on highly resolved microgeometries typically incur high computational costs, especially when three-dimensional models are used.

METHODS

The model microgeometries underlying the present study are space filling periodically repeating arrangements of identical spherical carbides embedded in a matrix, 15 of which are randomly positioned in three-dimensional unit cells. Appropriate particle positions were generated by a Random Sequential Adsorption algorithm, compare e.g. [15], modified to support periodic geometries. Typical unit cells of this type can be seen in Fig. 3. Despite the rather small number of particles involved, such models closely approach overall isotropic behavior in the elastic range, compare [11]. Even though the use of such microgeometries obviously involves a considerable degree of idealization, they are thought to be fairly realistic descriptions for the arrangements of carbides in tool steels produced by powder metallurgical routes.

The thermomechanical responses of the unit cells were evaluated by the Finite Element method, the preprocessor MSC/PATRAN V.8.5 (MacNeal–Schwendler Corp., Los Angeles, CA, 1998) and the analysis code ABAQUS V5.8/Standard (Hibbit, Karlsson and Sorensen Inc., Pawtucket, RI., 1998) being employed. The models were meshed with 10-node tetrahedral elements, periodic boundary conditions were enforced by appropriate constraint equations, and material as well as geometrical nonlinearities were accounted for. Element counts were of the order of 50,000 per unit cell.

The constituent material laws used in the analyses correspond to isotropic thermoelastic carbides embedded in an isotropic thermoplastic steel matrix described by a $J_2$ continuum plasticity model. The strain hardening of the matrix was approximated by a modified Ludwik hardening law.
\[ \sigma_y = \sigma_{y,0} + h \varepsilon_{\text{eqv},p}^n, \quad (1) \]

where \( h \) and \( n \) are the hardening coefficient and the hardening exponent, respectively, \( \sigma_y \) and \( \sigma_{y,0} \) represent the actual flow stress and the initial yield stress of the matrix, and \( \varepsilon_{\text{eqv},p} \) stands for the accumulated equivalent plastic strain. Because no data were available for the temperature dependence of the material parameters of matrix and carbides the same material behavior was employed for the whole temperature range considered; this approximation tends to overestimate thermal residual stresses and to underestimate plastic strains in the cooled-down HSS. The interfaces between the constituents were assumed to be perfectly bonded. Generic material parameters which had been used for modeling DIN S6–5–2–5 HSSs in a number of previous studies, compare e.g. [5, 14], were employed, see Table 1.

<table>
<thead>
<tr>
<th></th>
<th>( E ) [GPa]</th>
<th>( \nu )</th>
<th>( \sigma_{y,0} ) [GPa]</th>
<th>( h )</th>
<th>( n )</th>
<th>( m )</th>
<th>( \sigma_t ) [GPa]</th>
<th>( \alpha ) [K(^{-1})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel matrix</td>
<td>210</td>
<td>0.30</td>
<td>2.75</td>
<td>1.5</td>
<td>0.50</td>
<td>—</td>
<td>—</td>
<td>14.0 \times 10^{-6}</td>
</tr>
<tr>
<td>Primary carbides</td>
<td>450</td>
<td>0.25</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>5</td>
<td>3.66</td>
<td>6.0 \times 10^{-6}</td>
</tr>
</tbody>
</table>

The results of the Finite Element analyses were evaluated, on the one hand, in terms of homogenized material properties such as overall strain vs. temperature and stress vs. strain curves as well as effective moduli and effective coefficients of thermal expansion. On the other hand, the microscale distributions of the stresses and strains within the unit cells were described in terms of phase averages and the corresponding standard deviations. The evaluation of the latter type of results was based on an option of ABAQUS that allows the volume corresponding to each integration point to be output, so that the phase average of some function \( f \) can be approximated as
\[
< f > = \frac{1}{V_j} \int_{V_j} f(r) dV \approx \frac{1}{V_j} \sum_{l=1}^{N_j} f_l V_l \quad \text{with} \quad \sum_{l=1}^{N_j} V_l = V_j .
\]  

(2)

Here \( f_l \) and \( V_l \) are the function value and the integration weight (in terms of a volume), respectively, associated with the \( l \)-th integration point within a given phase \( (j) \), which contains a total of \( N_j \) integration points.

The failure relevant loads on the carbides were assessed by a modified Weibull concept [16], in which for a given loading condition each particle is assigned a fracture probability, \( P_i \), of the form

\[
P_i = 1 - \exp \left[ -\frac{1}{V_0} \int_{V_i : \sigma_1(r) > 0} \left( \frac{\sigma_1(r)}{\sigma_f} \right)^m dV \right] .
\]  

(3)

In this expression \( \sigma_1(r) \) stands for the spatial distribution of the maximum principal stress within the \( i \)-th carbide as obtained by the micromechanical analyses, \( V_i : \sigma_1(r) > 0 \) denotes the region of the particle for which this maximum principal stress is tensile, \( V_0 \) is a reference volume that was set equal to the carbides’ volume for the present study, while \( m \) and \( \sigma_f \) are the Weibull modulus and the characteristic strength of the particles. The values used for the latter two parameters are listed in Table 1. Equation (3) was evaluated by the approximate quadrature scheme given in eqn. (2).

It is worth noting that for the model described above the damage-free thermoelastoplastic material behavior does not depend on the absolute size of the carbides; such size effects must be explicitly introduced by an appropriate choice of the elastoplastic material parameters. The particle fracture probabilities, in contrast, show such a dependence because eqn. (3) intrinsically gives rise to higher values of \( P_i \) when \( V_l \) is increased. For a broader discussion of modeling issues in the use of three-dimensional multi-particle unit cell models see e.g. [11, 12]. Additional information on Weibull models for brittle particles embedded in a ductile matrix is given in [17].

**DISCUSSION OF RESULTS**

The thermal residual stresses in the model tool steel were evaluated for cooling down from a stress free temperature of 600 \(^\circ\)C to room temperature. All predictions in this section pertain to a carbide volume fraction of \( \xi = 0.15 \).
Most of the results presented in the following were obtained by ensemble averaging over a number of runs.

**RESIDUAL STRESS STATE**

Figure 1 depicts the predicted microscale von Mises equivalent residual stresses in the steel matrix after the cooling down process. The stress levels are grey coded on three parallel section planes within the unit cell, with dark shades of grey corresponding to high stress levels. A highly inhomogeneous distribution of the residual stresses is clearly evident, the lower coefficient of thermal expansion of the carbides giving rise to approximately concentric regions of elevated tensile hoop stresses and compressive radial stresses around each particle. Marked local stress maxima typically develop between closely approaching carbides.

In Table 2 predictions for the microscale von Mises equivalent stress, $\sigma_{\text{equiv}}$, the maximum principal stress, $\sigma_1$, the mean (hydrostatic) stress, $\sigma_m$.

![Figure 1](image.png)

*Figure 1.* Predicted residual von Mises equivalent stress in a tool steel cooled down from a stress free temperature of 600 $^\circ$C to room temperature.
and the accumulated equivalent plastic strain, $\varepsilon_{\text{eqv, p}}$, are listed in terms of phase averages $\pm$ the corresponding standard deviations for matrix ($m$) and carbides ($p$). The phase averaged equivalent stress in the matrix can be seen to reach about 18% of the initial yield stress, but the strong inhomogeneity evidenced by the large standard deviations nevertheless leads to a small amount of local yielding, which gives rise to a nonzero value of the phase average of $\varepsilon_{\text{eqv, p}}$. As expected, the phase averages of the mean stress are tensile in the matrix and compressive in the carbides, the absolute value being about 5 times higher in the latter on account of the phase volume fractions. Interestingly the standard deviations of the mean stress are relatively small in both constituents.

Table 2. Predicted residual state in a tool steel ($\xi=0.15$) cooled down from a stress-free temperature of 600 $^\circ$C to room temperature

<table>
<thead>
<tr>
<th>$\sigma_{\text{eqv}}^{(m)}$ [GPa]</th>
<th>$\sigma_m$ [GPa]</th>
<th>$\varepsilon_{\text{eqv, p}}$ [$\times 10^{-6}$]</th>
<th>$\sigma_{\text{eqv}}^{(p)}$ [GPa]</th>
<th>$\sigma_p$ [GPa]</th>
<th>$\varepsilon_{\text{eqv}}^{(m)}$ [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.50±0.36</td>
<td>0.16±0.02</td>
<td>0.02±3.97</td>
<td>0.31±0.19</td>
<td>-0.78±0.06</td>
<td>-0.92±0.02</td>
</tr>
</tbody>
</table>

For assessing the influence of changes in the material parameters it is worth noting that in general the magnitude of the self equilibrated residual stresses in a particle reinforced material subjected to cooling down grows with increasing temperature difference, with increasing thermal expansion mismatch between carbides and matrix, and with increasing matrix yield stress. Finally, it should also be mentioned that the effective coefficient of thermal expansion of the HSS was evaluated from the unit cells as $\alpha^*=1.26 \times 10^{-5}$K$^{-1}$, which is identical to results obtained from the Mori–Tanaka mean field theory [18].

INFLUENCE OF THE RESIDUAL STRESS STATE ON THE UNIAXIAL MECHANICAL BEHAVIOR

In a further step, the mechanical responses under uniaxial tensile loading up to an applied stress 3.0 GPa (which exceeds the initial yield stress of the matrix by about 9%) were simulated for an initially stress free (“virgin”) HSS and for a cooled-down HSS. The latter case corresponds to the “as
cooled-down” condition, i.e. possible reductions of the residual stress due to relaxation are not accounted for.

In Fig. 2 the predicted tangent moduli (obtained by differentiating the stress vs. strain curves) for the two cases are shown as functions of the applied stress. With the exception of some very minor differences at applied stresses between 2.5 GPa and 2.8 GPa, where progressive yielding of the steel matrix occurs, the curves are essentially identical and the effective Young’s modulus has a value of approximately 235 GPa in both cases. Evidently the simulations indicate that the thermal residual stresses have no significant influence on the uniaxial tensile response of HSSs. This result is in contrast to predictions from two-dimensional unit cell analyses, which cannot adequately account for the out-of-plane constraint and tend to show a noticeable influence of the residual stress state on the stress vs. strain response [19].

Table 3 lists predictions for some phase averaged microfields in virgin and cooled-down HSSs subjected to a tensile uniaxial stress of 3.0 GPa.

Only minor differences are present in the results for the matrix, the equivalent and mean stresses and the equivalent plastic strain being a few percent higher in the cooled-down case. The maximum principal stress and the mean stress in the particles, however, are predicted to be approximately 10% and 70% higher, respectively, in the virgin HSS. The former difference also translates into a small but noticeable reduction of the Weibull fracture probabilities of the particles in the cooled-down HSS. This effect can be seen in Fig. 3, which displays the predicted fracture probabilities of the individual carbides under uniaxial tensile loading in the $x$-direction, higher values of $P_i$ being indicated by darker shades of grey. It should be noted that these plots are strictly for simplified comparisons between virgin and cooled-down HSSs only — when particle fracture is accounted for in micromechanical models on the basis of Weibull statistics, the majority of particles do not reach fracture probabilities much beyond 0.5 before failing, see e.g. [3, 20], and the failure of individual particles leads to stress redistribution within the unit cell.

From the above results on the microfields some tendency can be discerned for particle fracture as well as interfacial decohesion to be somewhat more likely for the virgin material, whereas cooled-down HSSs are slightly more susceptible to damage initiation in the matrix. The predicted differences appear to be, however, too small to be of practical relevance.
Figure 2. Predicted effective tangent moduli as functions of the applied uniaxial tensile stress of a virgin (solid line) and a cooled down (dotted line) tool steel.

Figure 3. Weibull fracture probabilities of the carbides under a uniaxial tensile stress of 3 GPa acting in x-direction predicted for a virgin (top) and a cooled down (bottom) tool steel.
It is worth noting that much stronger effects of thermal residual stresses are present in aluminum based MMCs of similar particle volume fractions. Due to the much lower yield strength of the aluminum matrix and to the more marked elastic and thermal expansion contrasts between matrix and particles, cooling down by 380 °C suffices to cause essentially total yielding of the matrix. If stress relaxation effects are again neglected, there is no strictly elastic regime during subsequent uniaxial tensile loading of the cooled-down MMC, which shows a considerably reduced stiffness under uniaxial tensile loading, compare [21]. In analogy, tool steels with a lower matrix yield strength than the one given in Table 1 can be expected to show a stronger, but still rather limited sensitivity to thermal residual stress effects.

CONCLUSIONS

A three-dimensional Finite Element based multi-particle unit cell model was used to study the effects of thermal residual stresses from cooling down processes on the overall mechanical behavior of high speed tool steels. The results indicate that the stiffness and strength of HSSs are rather insensitive to such stresses, mainly due to the high initial yield stress of the steel matrix.

The main practical difficulties in using the above multi-particle modeling strategy lie in obtaining appropriate material parameters and in the high requirements in computational resources. The approach, however, allows for a considerable degree of flexibility in that different particle volume fractions and reinforcement shapes can be handled, see e.g. [22], a wide range of load cases and constituent material properties can be considered, and descriptions for progressive local damage, compare e.g. [3, 20], can be introduced.

ACKNOWLEDGMENTS

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REFERENCES

Table 3. Comparison of predicted microfields in virgin and cooled down tool steels (ζ≡0.15) subjected to a uniaxial tensile stress of 3 GPa

<table>
<thead>
<tr>
<th></th>
<th>$\sigma_{\text{eqv}}^{(m)}$ [GPa]</th>
<th>$\sigma_{\text{eqv}}^{(p)}$ [GPa]</th>
<th>$\varepsilon_{\text{eqv-st}}^{(m)} \times 10^{-2}$</th>
<th>$\sigma_{\text{ev}}^{(m)}$ [GPa]</th>
<th>$\sigma_{\text{ev}}^{(p)}$ [GPa]</th>
<th>$\sigma_{\text{eqv}}^{(p)}$ [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>virgin</td>
<td>2.87±0.05</td>
<td>1.03±0.27</td>
<td>0.77±0.38</td>
<td>4.31±0.23</td>
<td>3.80±0.22</td>
<td>0.94±0.13</td>
</tr>
<tr>
<td>cooled down</td>
<td>2.88±0.04</td>
<td>1.09±0.25</td>
<td>0.81±0.38</td>
<td>4.40±0.22</td>
<td>3.48±0.23</td>
<td>0.55±0.15</td>
</tr>
</tbody>
</table>