Finite Element Simulation of Surface Microstructure Effects in Metal Cutting

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Abstract: During a machining process, the severe temperature and deformation experienced by the surface layer of a workpiece can cause changes in microstructure, commonly known as “white layer” formation. These surface changes can result from recrystallization or from phase changes in the base material. It is generally desirable to avoid these changes due to their adverse influence on fatigue life. The affected surface layer is also frequently harder than the base material, and as such may adversely influence machinability in subsequent operations.

Cutting speed, rake angle, tool edge preparation, tool wear, and coolant all play a role in surface microstructure changes. Commercially available finite element simulation software (DEFORM) which contains extensively developed microstructure models, has been used to study the effect of these parameters during cutting. New phases, grain sizes, percentage recrystallization, and other microstructure details are derived from stress, strain, and temperature evolution through the workpiece. Depending on models used, the updated microstructure can influence process behavior as the simulation continues. In this article, a comparison is made between simulation results and previously published experimental data.

Keywords: Machining, White Layer, Microstructure, Hard Turning, Martensite

1 INTRODUCTION

High performance cutting of hardened steels can challenge the surface integrity of the workpiece. The disturbance of surface microstructure can have an adverse effect on product performance, and thus avoiding this condition becomes a limiting factor in cutting process performance.

Finite element simulation of metal cutting processes has been a popular research topic since the mid 1990’s. In more recent years, increasing industrial applications have been reported with commercially available simulation software. Simulation has proven a useful tool for prediction of cutting tool performance, chip control, temperature, cutting forces, and other important variables [Fischer et. al. 2006], [Kammermeier, et. al. 2006].
Many researchers are reporting successful results with residual stress prediction using commercial software. However, simulation of surface microstructure effects using commercial software has proven challenging.

Certain machining conditions are known to produce a cut surface layer commonly known as “white layer.” This layer – so called because of its appearance in a micrograph after etching – is problematic for part performance because it can adversely affect fatigue life. Ramesh [Ramesh 2002] used the commercial finite element code ABAQUS Explicit to simulate microstructure effects. His work was only possible with substantial modifications to the software through user developed subroutines describing transformation kinetics. While this sort of research is ideal for development of fundamental theory, it is difficult to transfer this technology into industry.

The purpose of the present investigation is to study the capabilities of unmodified, commercially available software to predict microstructure changes associated with white layer.

2 PRIOR RESEARCH

Ramesh [2002] cites Griffiths [Griffiths 1987] in proposing three mechanisms for white layer formation:

1) Rapid heating of ferrous alloys to above the austenite start temperature, followed by cooling rapid enough to form martensite
2) Grain refinement due to strain, temperature, and stress induced recrystallization
3) Accelerated surface reaction with the environment due to elevated temperatures.

The present research will focus on the austenite/martensite mechanism, which is believed to be the primary mechanism for white layer formation in high speed machining of steels [Ramesh 2002]. Another group of researchers are concurrently studying the recrystallization mechanism [el-Wardany et. al. 2008], which is believed to be dominant in nickel based superalloys, among other materials.

Ramesh used ABAQUS Explicit for Lagrangian finite element analysis of surface behavior, including extensively developed VUMAT FORTRAN subroutines, not only for transformation models, but also for basic elastic-plastic constitutive behavior. The research noted that the software does not include automated remeshing, so a pre-defined separation plane is required.

Han [Han 2006] performed experiments on several materials, including AISI 52100 (equivalent to DIN 100Cr6) and reported white layer details, including measured depth and microhardness measurements. The research used commercially available finite element software (AdvantEdge) to predict surface temperatures, but did not include microstructure predictions in the finite element model. This present study will attempt to
duplicate Han’s results, including microstructure and hardness behavior, using unmodified software with published input data.

3 MATERIAL MODELING IN COMMERCIAL SOFTWARE.

3.1 Microstructure Model
Arimoto [Arimoto et. al. 1998] reported on the development of microstructure models as part of the structure of DEFORM finite element software. The software includes coupled mechanical, thermal, and microstructure analysis.

The diffusion and martensitic types of phase transformation are modeled. The system is designed for both ferrous and nonferrous metals. Using carbon steel as an example, the austenite-ferrite and austenite-pearlite structure changes and vice versa are governed by the diffusion type transformation. The transformation is driven by a diffusion process depending on the temperature, stress history, and carbon content. The diffusionless transformation from the austenite to martensite involves a shear process which depends on the temperature, stress, and carbon content.

Material properties are determined by a mixture rule on an element by element basis.

\[ \Phi = \sum_i \xi_i \phi_i \]  

where \( \Phi \) is the aggregate property for the element (e.g., flow stress, thermal conductivity, etc), \( \phi_i \) is the corresponding property for the \( i \)th phase, and \( \xi_i \) is the volume fraction of the \( i \)th phase for a given element.

During Lagrangian analysis, at each time step, the phase volume fractions are calculated based on temperature and deformation results from that step. The updated properties are then used for the deformation and temperature calculations at the next step. Diffusion and diffusionless type transformations are modeled from typical transformation curves.

3.1.1 Diffusion type transformations
For the Johnson-Mehl equation, one of the most popular kinetic equations is of the form:

\[ \xi = 1 - \exp(-bt^n) \]  

where \( \xi \) is the volume fraction of product phase, \( t \) is the time, and \( b \) and \( n \) are material constants defining the transformation. Using this equation, the transformation can be defined by a table representation of a Time-Temperature-Transformation (T-T-T) diagram. Transformation begins for a given element after the incubation time has been reached for that element and progresses according to start and end times in the TTT diagrams.

3.1.2 Diffusionless type (martensitic) transformations
Magee’s equation [Magee 1968] is used to describe the diffusionless-type transformation. The volume fraction of martensite \( \xi_M \) is obtained by:
\[ \xi_M = 1 - \exp \left\{ \psi_1 T + \psi_2 \left( C - C_0 \right) + \psi_3 \sigma_m + \psi_4 \sigma^{1/2} + \psi_4 \right\} \]  \hspace{1cm} (3)

Where \( \psi_1, \psi_2, \psi_{31}, \psi_{32}, \) and \( \psi_4 \) are material constants, \( \sigma_m \) is the mean stress, \( \sigma \) is the effective stress, \( C \) the carbon content, \( C_0 \) the initial carbon content. If temperatures under carburized conditions and the applied stress field are given, \( \psi_2/\psi_1, \psi_{31}/\psi_1, \) and \( \psi_{32}/\psi_1 \) can be determined, and \( \psi_1 \) and \( \psi_4 \) are identified if temperatures for martensite-start \( T_{MS} \) and for 50% martensite \( T_{M50} \) at \( \xi_M = 0 \) and \( \xi_M = 0.5 \) are provided.

### 3.1.3 Recrystallization and grain growth

With a slightly different form

\[ \Phi = 1 - \exp \left\{ - b \left( \frac{t}{t_{0.5}} \right)^n \right\} \]  \hspace{1cm} (4)

recrystallization can be modelled, where \( t_{0.5} \) is the time for 50% recrystallization which is described by the equation

\[ t_{0.5} = a \varepsilon^m d_0^n \exp \left( \frac{Q}{RT} \right), \]  \hspace{1cm} (5)

where \( a, m, \) and \( n \) are material constant, \( Q \) is activation energy, \( R \) is universal gas constant, \( T \) is absolute temperature, \( \varepsilon \) is prior plastic strain obtained after an operation of forming and \( d_0 \) is an initial grain size. The grain growth model takes the form

\[ d^{n1} - d_0^{n2} = K t^{n3} \]  \hspace{1cm} (6)

where \( n1, n2, n3, \) and \( K \) are material constants, \( d_0 \) is the original grain size.

### 3.2 Heat Transfer Model

The temperature field is governed by the Laplace equation:

\[ \rho \varepsilon \dot{T} = \frac{\partial}{\partial X} \left( K \frac{\partial T}{\partial X} \right) - \eta \sigma_{ij} \dot{e}_{ij} + L_I \dot{\xi}_I + \dot{Q} \]  \hspace{1cm} (7)

where \( \rho, c, K \) and \( L_I \) denote density, specific heat, heat conduction coefficient and the latent heat produced by the progressive \( I \)-th constituent with volume fraction \( \xi_I \), respectively. The 2nd, 3rd and 4th terms represent the heat due to plastic deformation, the latent heat absorbed or released during the phase transformation, and the heat source such as eddy current during induction heating. For plastic deformation, a deformation efficiency term \( \eta \), typically taken to be 0.9, relates plastic deformation energy to heat energy.

To accommodate the complex thermal boundary condition during the heating/cooling processes, the heat transfer coefficient can be specified not only as a function of surface temperature, but also as a function of surface location.
3.3 Deformation Model
The same mixture rule used for the thermal material data is used for all elastic and plastic material data. The incremental strain is assumed to consist of several components,

\[ d\varepsilon = d\varepsilon^E + d\varepsilon^\theta + d\varepsilon^P + d\varepsilon^{Tr} + d\varepsilon^{Tp} + d\varepsilon^C \]  

(8)

where superscripts \( E, \theta, P, Tr, Tp, \) and \( C \) represent the entities for elastic, thermal, plastic, phase transformation, transformation plasticity, and creep[Inoue 1997].

When introducing a temperature and structure-dependent yield function with the hardening parameter \( \kappa, F = F(\varepsilon_{ij}, \varepsilon_{ij}, \kappa, T, \xi) \), the plastic strain rate, elastic strain rate, and thermal strain rate, can be expressed in the following form:

\[ \dot{\varepsilon}_{ij}^P = \lambda \frac{\partial F}{\partial \sigma_{ij}} \]

\[ \dot{\varepsilon}_{ij}^E = \frac{1+\nu}{E} \sigma_{ij} - \nu \frac{E}{\sigma_{kk}} \delta_{ij} \]

\[ \dot{\varepsilon}_{ij}^T = \alpha \left( T - T_0 \right) \xi_{ij} \]

(9)

where \( \lambda \) is a positive proportionality constant, \( \nu \) is the Poisson ratio, \( E \) is the Young’s modulus, \( \delta_{ij} \) is the Kronecker’s delta, \( T \) is the temperature, \( T_0 \) is the temperature of the previous step, and \( \alpha \) is the thermal expansion coefficient.

During the heat treatment process, some phase transformations may take place. The phase transformations produce the material volume changes due to the metallic structure change. For example in carbon steel, the austenite structure is Face Centered Cubic (FCC), the pearlite is Body Centered Cubic (BCC) and the martensite is Body Centered Tetragonal (BCT). The transformation strain is used mainly to account for the structure change during the transformation and is in the form of:

\[ \dot{\varepsilon}_{ij}^{Tr} = \sum \beta_I \dot{\varepsilon}_I \delta_{ij} \]

(10)

Where \( \beta_I \) is the transformation strain coefficient from one phase to another, and \( \dot{\varepsilon}_I \) is transformation volume fraction rate.

4 COMPARISON OF SIMULATION AND EXPERIMENTAL RESULTS

4.1 White layer creation and measurement
Han performed experiments on 52100 tubes, oil quenched, and tempered at 316C for 2 hours to obtain a hardness of 53.5 +/- 0.8 HRC. The tubes had a wall thickness of 1.5 mm. With a feed of 0.1mm, orthogonal cutting conditions were achieved.
A PCBN tool with 0 degree rake angle was used. To ensure conditions which would generate white layer, hard material was cut to generate a uniform flank wear of 100µm. Experiments were performed with cutting speeds of 100 m/min and 300 m/min.

White layer depth was measured using optical micrographs. Nano-indentation hardness measurements were made through the workpiece surface layer and into the base layer after mounting and polishing the material sample at an oblique angle to better expose the thickness of the white layer.

The experimental results are reported in Table I.

<table>
<thead>
<tr>
<th>Speed (m/min)</th>
<th>Cutting Force (N)</th>
<th>Thrust Force (N)</th>
<th>White Layer Depth (µm)</th>
<th>White Layer Nano-hardness (GPa)</th>
<th>Bulk material Nano-hardness (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>350</td>
<td>425</td>
<td>4</td>
<td>9</td>
<td>6.5</td>
</tr>
<tr>
<td>300</td>
<td>300</td>
<td>400</td>
<td>5.5</td>
<td>10</td>
<td>6.5</td>
</tr>
</tbody>
</table>

4.2 Material

4.2.1 Flow Stress


\[
\sigma(\varepsilon, \dot{\varepsilon}, T, HRC) = B(T)(C\varepsilon^n + F + G\varepsilon)[1 + (\ln(\dot{\varepsilon}))^m - A] 
\]

(11)

Where the temperature softening multiplier \( B(T) \) is given by:

\[
B(T) = \exp(aT^5 + bT^4 + cT^3 + dT^2 + eT + f) 
\]

(12)

And the coefficients \( F \) and \( G \) in the strain hardening term are functions of hardness given by:

\[
\begin{align*}
F(HRC) &= 27.4HRC - 1700.2 \\
G(HRC) &= 4.48HRC - 279.9 
\end{align*} 
\]  

(13)
The authors reported the coefficients as:

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Coefficient</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>1092MPa</td>
<td>b</td>
<td>-3.2927e-12</td>
</tr>
<tr>
<td>n</td>
<td>0.083</td>
<td>c</td>
<td>-6.9118e-9</td>
</tr>
<tr>
<td>A</td>
<td>0.0567</td>
<td>d</td>
<td>5.4993e-6</td>
</tr>
<tr>
<td>m</td>
<td>0.1259</td>
<td>e</td>
<td>-1.2419e-3</td>
</tr>
<tr>
<td>a</td>
<td>3.8121e-15</td>
<td>f</td>
<td>0.02443</td>
</tr>
</tbody>
</table>

Curves were calculated for these values for a hardness of 53.5HRC over a strain rate range of 1 to 1e6, a temperature range of 20-1000°C, and a strain range of 0-5, in an Excel™ spreadsheet, and entered into the DEFORM flow stress model in tabular form.

Chip segmentation effects, which are known to occur in hardened materials, were neglected for numerical convenience. Ramesh [Ramesh et. al. 2003] and Guo and Liu[Guo 2002] have shown that this assumption does not influence surface behavior.

4.2.2 Microstructure and Transformation Kinetics

The simulation attempts to capture transformation due to thermal, stress, and strain effects in a material layer which is a few microns thick. Accurate modeling of transformation kinetics is essential for good agreement with experimental results. The critical values are initial microstructure phase volume fraction, austenite transformation, and martensite transformation.

Using a hardness vs. time and tempering temperature chart from Calister [Calister 2003], and phase hardness estimates from the DEFORM material library, a mixture rule approach was used to estimate a volume fraction ratio of 68% martensite (at a phase hardness of 65HRC), 32% BCC ferrite+carbide (phase hardness of 30 HRC). Subsequent literature reviews confirmed the estimated 70% phase volume fraction martensite. Based on these estimates, the simulation model was initialized with a 68% volume fraction martensite, 32% volume fraction pearlite.

The nominal austenite start temperature for AISI 52100 is 732°C. Ramesh [Ramesh 2002] calculated the influence of stress and strain on the austenite start temperature. He estimated that the applied stress resulted in a reduction in start temperature of 112°C. The high dislocation density associated with large strain creates nucleation sites for incipient austenite grains. Based on experimental work and theoretical calculations, he determined a further reduction for strain, resulting in an approximate austenite start temperature of 550°C.

An Avrami type equation is used for austenite transformation in DEFORM. The volume fraction of austenite is given by:

$$\xi_A = 1 - \exp\left\{-4\left(\frac{T - T_s}{T_f - T_s}\right)^2\right\}$$  \hspace{1cm} (14)
The latent heat of transformation, from the DEFORM material library, is -661.51 N/mm² for Martensite->Austenite and -595.36 N/mm² for Pearlite->Austenite.

Martensite transformation is defined by the McGee equation, where the volume fraction martensite is given by:

\[ \xi_m = 1 - \exp \left( 0.016T - 0.001223\sigma_m - 0.0010303\sigma - 5.18 \right). \]  

(15)

Hardness estimates in DEFORM are based on phase volume fractions, with martensite phase at 65HRC and Ferrite+Carbide (Pearlite or Banite) at 30HRC.

Default thermal properties from the DEFORM material library for AISI52100 were used.

4.3 Simulation Results

A workpiece segment 1.5mm long and 1mm thick was used in DEFORM. Given the expected thickness of the white layer, a minimum element size of 1.5µm was specified along the cut surface of the workpiece. A default convection coefficient of 0.02 N/(s.mm.C) – representative of still air - was used along the surface of the workpiece.

The tool geometry had 0° face rake, 5° flank rake. As noted in the experimental work, the tool was pre-worn to 100µm flank wear to generate conditions for abusive cutting. This flank wear was modeled along with a 10µm radius on the cutting edge.

A thermal conductivity of 20 N/s.C was used for the CBN tool. A fixed temperature of 20°C was used on the back side of the tool. A constant shear friction factor of 0.6 and a contact heat transfer coefficient of 45 N/(s.mm.C) were used.

An 0.1mm uncut chip thickness was modeled using a plane strain assumption. Two cuts were made, with a time dwell between cuts consistent with 1 revolution of the tube used for experiments. The first cut was to establish a temperature profile in the workpiece. The second was to study microstructure response. After the 2nd cut was completed, the part was simulated air cooling to 30°C, to allow transformation to complete.
4.3.1 White Layer Thickness

The white layer thickness was measured from the contour plots of the simulation as shown in figures 1, 2, and 3. Figure 4 shows a comparison of the measured values reported by Han [Han 2006] and the DEFORM simulation under the same conditions. Agreement between predicted and measured values is quite good.
Figure 2: Detail of simulation results of cut workpiece surface for 100 m/min cutting speed. Light gray region is base tempered martensite (68%) with ferrite and carbide (32%). Darker regions indicate increasing volume fractions of martensite.
Figure 3: Detail of surface martensite for 300m/min simulation. Note increased martensite thickness over figure 2.

Figure 4: Comparison of measured and simulated white layer thickness for 100m/min and 300 m/min cutting speeds.
4.3.2 Hardness

DEFORM hardness estimates are based on phase volume fractions and relative hardnesses of the constituent phases. The hardness as a function of distance from the surface is shown in Figure 5. Two experimental data points reported by Han are included in the chart. The white layer hardness was reported as a nano-hardness value. To correlate this value with Rockwell C scale measurements and DEFORM predictions, data from Mencin et. al. [Mencin] was used to fit a regression equation:

\[
HRC = \frac{mh - 0.3085}{0.1416} \tag{16}
\]

Where \( mh \) is the microhardness. For a measured microhardness of 9.3GPa, this equation predicts a Rockwell hardness of 62.5HRC.

![Figure 5: Simulation results (square, small circle) and experimental measurements (large circles) of hardness as a function of distance from the cut surface. The near surface experimental value was calculated from nano-indentation measurements as described in the text.](image)
5 CONCLUSIONS

Simulations of white layer formation in AISI 52100 were performed using unmodified, commercially available software with published experimental data. The results showed excellent agreement in both white layer thickness and hardness. This capability in a relatively easy to use software package makes application of this technology feasible for industrial application, not just academic research.

This paper addresses one of three theorized mechanisms of white layer formation, namely austenitization of the surface layer and subsequent martensite formation due to rapid cooling. Further research is needed for recrystallization and surface reaction effects.

6 REFERENCES


[El Wardany 2008] El Wardany, T; Pifiefer, C; personal communication with the author.


