Original Article

Dislocation density and grain size evolution in hard machining of H13 steel: numerical and experimental investigation

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ABSTRACT

In this research, the microstructure evolution in the machined subsurface is numerically simulated through a developed multi-physics model applied to H13 hot work die steel. The multi-physics model based on dislocation density evolution is utilized to predict the change of grain size through finite element analysis by varying cutting parameters. In spite of the cutting conditions, the simulated grain size on the top-most machined surface is around 330 nm, and the machining-affected depth with refined grain varies in the range of 25–45 μm. In addition, the appeared periodical fluctuation of dislocation density and grain size in a wavy configuration induced by the generated serrated chip segments is revealed. The efficacy of the proposed finite element model is verified and the probable mechanism of grain refinement is demonstrated with the assistance of TEM observation, which in turn promotes the in-depth understanding of microstructure evolution during metal cutting.

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1. Introduction

Hot-working dies steel is commonly applied to manufacture die mold and casting, which serves under high pressure and temperature due to the attractive mechanical properties. Among all the failure modes, thermal cracking is mainly responsible for the limited service life of the die casting [1]. Furthermore, it should be highlighted that the thermal cracking induced by periodical heating and cooling during service is frequently observed initiating from the machined surface and then progressively propagates leading to the final failure of the components [2]. Consequently, the metallurgical states of the surface layer play a crucial role in determining the macro-level mechanical property and thus affects its functional performance. Usually, the depth of the machining-affected layer varies from several microns up to a few hundred microns.

Currently, hard machining has been successfully applied to dry milling of hardened steels. As far as hard machining is concerned, the investigations that focus on surface geometrical states [3,4] and hard machining mechanics [5,6] have been achieved substantial progress. Wojciechowski et al. [7] evaluated the relationship between surface roughness and the instantaneous tool displacement when precise ball-end milling of hardened alloy steel. Pradhan et al. [8] investi-
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Nomenclature

A, B, n, C, m JC model parameters
\( \sigma \) plastic flow stress
\( \dot{\varepsilon} \) strain rate
\( T_{fs} \) transition temperature
\( \dot{\varepsilon}_{fs} \) strain at failure
\( \sigma^*, \beta^*, \kappa_0 \) dislocation evolution rate control parameters
\( d \) dislocation cell size
\( n \) temperature sensitivity
\( f \) volume fraction of cell wall
\( b \) magnitude of the Burgers vector
\( \xi \) fraction of dislocation into cell walls from cell interiors

\( M \) Taylor factor
\( \dot{\gamma}^{c} \) shear strain rate
\( \dot{\gamma}^{w} \) shear strain rate in cell wall
\( \dot{\gamma}^{i} \) shear strain rate in the cell interior

\( \dot{\gamma} \) von Mises strain rate
\( \rho_{dis} \) initial dislocation density
\( R \) universal gas constant
\( d_1-d_3 \) JC shear damage model parameters
\( \varepsilon \) equivalent plastic strain
\( \dot{\varepsilon}_0 \) reference strain rate
\( T_m \) melting temperature
\( \tilde{\theta} \) non-dimensional temperature
\( \gamma^{c} \) shear strain
\( \gamma^{i} \) reference shear strain
\( \rho_c \) cell interior dislocation
\( \rho_w \) cell wall dislocation
\( \rho_{wa} \) statistical density
\( \rho_{wg} \) geometrically necessary dislocation
\( \rho_{tot} \) total dislocation density
\( T \) temperature

\( K \) material coefficient
\( M_k \) martensite transformation temperature (K)
\( Q_0 \) activation energy for motion of vacancies
\( C_{dis} \) material constant

The objective of this research is to model grain refinement during hard milling of H13 steel with a multi-physics material model under different cutting parameters. Special attention is paid to the impact of serrated chip formation on grain size distribution on the machined surface. The multi-physics model is verified by microstructural observation for experimental samples under TEM to demonstrate the grain refinement.
2. Numerical model and experimental procedures

2.1. Constitutive model

The Johnson–Cook (JC) constitutive model (Eq. (1)) and JC shear failure criterion (Eq. (2)) were respectively used to describe the material plasticity behavior and chip formation in the milling of H13 steel. The workpiece was provided by The thermomechanical coupled 2D FE milling model was validated in the authors’ previous research [23,24] with given material constants for the FE model of H13 steel.

\[
\sigma = (A + B\varepsilon^n) \left[ 1 + C \ln \left( \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right) \right] \left[ 1 - \left( \frac{T - T_r}{T - T_m} \right)^m \right]
\]

\[
\dot{\varepsilon}_p^\text{pl} = \left( d_1 + d_2 \exp (-d_3 \eta) \right) \left( 1 + d_4 \ln \left( \frac{\dot{\varepsilon}_p^\text{pl}}{\dot{\varepsilon}_0} \right) \right) \left( 1 - d_5 \tilde{\varepsilon} \right)
\]

2.2. Dislocation density-based material model

The dislocation density-based model is firstly proposed by Estrin [25] to describe the hardening behavior of cellular crystalline material at large strain deformation like torsion. Afterward, Ding and Shin [26,27] adapted the dislocation density-based plasticity model to model the surface microstructure alteration and grain refinement in orthogonal cutting of titanium and AISI 52100 steel. Wang et al. [28] investigated the microstructure evolution of tempered H13 steel during high temperature tensile and observed dislocation density, subgrain as well as twinning behavior, which presents the similarity with hard machining involving high temperature and shear deformation.

In the following, a brief description of the dislocation density-based plasticity model used for grain size prediction is introduced. It is assumed that cellular substructure is going to be generated during material plastic deformation. According to the previously developed model, a cellular dislocation structure consists of cell walls and cell interiors [26]. The corresponding dislocation density evolution can be divided into two parts: the cell interior dislocation \( \rho_c \) and the cell wall dislocation \( \rho_w \). More in detail, the cell wall dislocation density also consists of the geometrically necessary dislocation density \( \rho_{w0} \) and the statistical dislocation density \( \rho_{ws} \). Their evolution rates can be calculated by the following equations:

\[
\dot{\rho}_c = \alpha^* \frac{1}{\sqrt{3}b} \sqrt{\rho_{w0} \dot{\rho}_w} - \beta^* \frac{6}{bd(1-f)^{1/3}} \dot{\varepsilon}^\text{pl} - k_0 \left( \frac{\dot{\varepsilon}_c}{\dot{\varepsilon}_0} \right)^{-\frac{1}{n}} \rho_c \tilde{\varepsilon}^\text{pl}
\]

\[
\dot{\rho}_{w0} = \delta \beta^* \frac{6}{bd(1-f)^{1/3}} \dot{\varepsilon}^\text{pl}
\]

\[
\dot{\rho}_{ws} = \beta^* \frac{\sqrt{3}(1-f)}{f_b} \sqrt{\rho_{w0} \dot{\rho}_w} + (1 - \delta) \beta^* \frac{6(1-f)^{2/3}}{bd} \dot{\varepsilon}^\text{pl} - k_0 \left( \frac{\dot{\varepsilon}_w}{\dot{\varepsilon}_0} \right)^{-\frac{1}{n}} \rho_{ws} \tilde{\varepsilon}^\text{pl}
\]

The strain compatibility requires the shear strain rate in the cell wall \( \dot{\varepsilon}_w \) and in the cell interior \( \dot{\varepsilon}_c \) is equal and satisfy the following equation:

\[
\dot{\varepsilon}_w = \dot{\varepsilon}_c = \dot{\gamma}^\text{pl}
\]

with resolve shear strain rate \( \dot{\gamma}^\text{pl} \):

\[
\dot{\gamma}^\text{pl} = M \dot{\varepsilon}^\text{pl}
\]

The temperature sensitivity \( n \) can be obtained:

\[
n = \frac{A}{T}
\]

The volume fraction of the cell wall dislocation density \( f \):

\[
f = f_\infty + (f_0 - f_\infty) e^{-\gamma/\dot{\varepsilon}^\text{pl}}
\]

The total dislocation density \( \rho_{tot} \) is assumed to obey the rule of mixture, can be written as:

\[
\rho_{tot} = f \rho_w + (1 - f) \rho_c
\]

Thus, the dislocation cellular substructure size \( d \) can be assessed:

\[
d = \frac{K}{\sqrt{\rho_{tot}}}
\]

The grain size in this dislocation density-based material model is considered to the cellular substructure under strain deformation, which is supposed to be the precursor of the fully developed grain.

In this present work, the experimental material H13 steel is subjected to multiple heat treatments including quenching and tempering. The steel microstructure consists only of tempered martensite. A general equation used to estimate the initial dislocation density \( \rho_{dis0} \) of martensite at room temperature after quenching depending on the martensite transformation start temperature \( M_s \), as proposed by Bhadeshia et al. [29].

\[
\log (\rho_{dis}) = 9.2840 + \frac{6880.73}{M_s} - \frac{1780.36}{M_s^2}
\]

During the tempering stage, the evolution of dislocation density inherited from the quenching stage is governed by an Arrhenius type equation [30]:

\[
\frac{d\rho_{dis}}{dt} = -C_{dis} \rho_{dis} \exp \left( \frac{-Q_v}{RT} \right)
\]

with \( C_{dis} \) is a constant (3.002 × 10^8) and \( R \) is the universal gas constant (8.3145 J mol^-1 K^-1).
Table 1 – Constants for dislocation density-based material model of H13 steel.

<table>
<thead>
<tr>
<th>$a^*$</th>
<th>$\beta^*$</th>
<th>$k_0$</th>
<th>$\lambda$</th>
<th>$n$</th>
<th>$f_0$</th>
<th>$f_{\infty}$</th>
<th>$M$</th>
<th>$K$</th>
<th>$\gamma$</th>
<th>$\rho_{\infty}$</th>
<th>$\rho_{0}$</th>
<th>$b$</th>
<th>$\alpha$</th>
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<tbody>
<tr>
<td>0.06</td>
<td>0.01</td>
<td>8.0</td>
<td>6e4</td>
<td>100</td>
<td>0.25</td>
<td>0.06</td>
<td>3.06</td>
<td>30</td>
<td>3.2</td>
<td>1e7</td>
<td>1e8</td>
<td>2.86e-7</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Fig. 1 – Flow chart for cutting simulation with implemented user subroutine.

The dislocation density-based material model was integrated into the FE cutting simulation model in Abaqus/Explicit programmed in FORTRAN as a VUSDFLD user subroutine. The simulation flow chart with implemented dislocation density-based user subroutine is shown in Fig. 1.

2.3. Hard milling experiment

The key hot working dies steel in manufacturing die casting, H13 steel, was investigated in this research. The nominal chemical compositions of H13 steel are listed in Table 2. To assess the multi-physics based model in prediction of grain size variation, three sets of peripheral milling experiments were conducted under dry condition using Ti(C, N)–Al₂O₃ coated cemented carbide cutting insert (Seco, XOMX090308TRM08, MP1500) with −10° rake angle, +15° clearance angle and 0.8 mm nose radius. The milling cutter with a diameter of 20 mm can be mechanically mounted with three milling inserts at one time. But only one insert used in order to eliminate tool wear effect. Detailed cutting parameters are listed in Table 3. The used experimental material before hard milling was subjected to multiple heat treatments including austenitization, quenching and tempering. The initial microstructure of H13 steel is tempered martensite with hardness about 50 HRC. Samples for TEM (JEOL, JEM-2100) observation were subjected to mechanical polishing until the thickness became less than 100 μm and subsequently apply focused ion beam (FIB) to keep thinning the sample to less than 50 nm for microstructure analysis. The thermo-mechanical properties of H13 steel can be found in Ref. [31].

3. Results and discussions

3.1. Simulation results

The simulated total dislocation density (SDV 15) and grain size (SDV 22) at different cutting conditions by using an integrated user-defined routine is presented. The initial grain size is associated with the dislocation density existing in the experimental material after tempering prior to milling. Based on Eq. (10), the initial grain size can be obtained with a size of about 1.14 μm, which is in agreement with the statistical grain size around 1-2 μm [32].

Table 2 – Nominal chemical composition of H13 steel (wt%).

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>Cr</th>
<th>Mo</th>
<th>V</th>
<th>P</th>
<th>S</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.32–0.45</td>
<td>0.8–1.25</td>
<td>0.2–0.6</td>
<td>4.75–5.5</td>
<td>1.1–1.75</td>
<td>0.8–1.2</td>
<td>≤0.03</td>
<td>≤0.03</td>
<td>Balance</td>
<td></td>
</tr>
</tbody>
</table>

Table 3 – Hard milling experimental condition for model verification.

<table>
<thead>
<tr>
<th>No.</th>
<th>v_c (m/min)</th>
<th>f_z (mm/rev)</th>
<th>a_e (mm)</th>
<th>a_p (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1#</td>
<td>300</td>
<td>0.2</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>2#</td>
<td>300</td>
<td>0.3</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>3#</td>
<td>300</td>
<td>0.2</td>
<td>3.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Fig. 2 – Simulated dislocation density (a, c, e) and grain size (b, d, f) by varying cutting speed (a, b) v_c = 200 m/min, f_z = 0.2 mm/rev, a_e = a_p = 2.0 mm, (c, d) v_c = 300 m/min, f_z = 0.2 mm/rev, a_e = a_p = 2.0 mm and (e, f) v_c = 400 m/min, f_z = 0.2 mm/rev, a_e = a_p = 2.0 mm.

3.1.1. Effect of cutting speed
The effect of cutting speed on dislocation density and grain size is shown in Fig. 2. It is apparent that the propagation and accumulation of the dislocation is mainly concentrated on three deformation zones, i.e., primary shear zone (shear band), secondary deformation zone (tool-chip contact surface) and tertiary deformation zone (machined surface layer). In this research, the metallurgical alteration in the machined subsurface is the main focus. With increasing cutting speed, the similarity among the predicted results is the distribution with a great gradient below the machined surface. Actually, the velocity of dislocation propagation in the metal cutting pro-

cess outstrips the cutting speed. Therefore, it can be observed in the contour maps that the dislocation accumulation zone is ahead of the cutting tool. In other words, the propagation and continuous mobility of dislocation under external force eventually lead to the shear plastic deformation. As illustrated in Fig. 2(a), path 1 and path 2 were created respectively along the top-most machined surface and the direction from the surface into the bulk material. Quantitative comparison including dislocation density and grain size under various cutting conditions is performed.

Fig. 3 illustrates the distribution of predicted dislocation density and grain size along path 1 and path 2 by varying cutting speed. Along path 1, the machined surface, the dislocation density fluctuates around $1.0 \times 10^6$ mm$^{-2}$ under all the three selected cutting speed without exhibiting significant disparity. However, several locations with higher dislocation density exceeding $2.0 \times 10^{10}$ mm$^{-2}$ at 200 and 300 m/min are highlighted. More in detail, the height of the several peaks gradually decreases with uncut chip thickness reduces. The appearance of high dislocation density location is assumed to be caused by the plastic deformation concentration resulted from periodical vibration due to serrated chip formation. Accordingly, the surface grain size can be obtained as shown in Fig. 3(b). The cutting speed has little impact on surface grain size variation with a grain size of approximately 330 nm. It is confirmed that the cutting temperature increases with cutting speed [33], the grain size on the machined surface varies little. This shows that grain refinement is dominantly strain-dependent [34]. The distribution trend is demonstrated in wavy shape continuously. The points with higher dislocation density are oppositely corresponding to smaller grain sizes, which reaches about 230 nm. Along path 2, the dislocation density distributions are very close to each other at cutting speed 200 and 300 m/min while presents a little increase at 400 m/min. As far as grain size is concerned, it reduces as cutting speed increasing with affected depth reaches about 40 μm. During the metal cutting process, higher cutting speed accompanying a high level of strain rate results in the decreases of deformation layer thickness [35]. As a consequence, an extremely short time under higher cutting speed is left for plastic deformation to occur deep into the subsurface. It should be pointed out that the predicted grain sizes within the affected layer less than 4 μm are almost the same under different cutting speeds. When the depth continues to increase, the distinction of grain size affected by varying cutting speed is highlighted.

3.1.2. Effect of feed

Fig. 4 shows the predicted distribution of dislocation density and grain size under different feed rates. The feed rate generates a visible effect on dislocation density along path 1 as shown in Fig. 5(a). The dislocation density accumulates from about $9.5 \times 10^8$ to $1.2 \times 10^9$ mm$^{-2}$ with feed rate increases from 0.1 to 0.3 mm/rev. With respect to feed rate increasing, an apparent rise in mechanical energy is required to shear the material [36]. Compared to the marginal change of grain size by varying cutting speed, Umbrello [11] also previously found that feed rate seems to be more predominant on grain refinement than cutting speed. Furthermore, the fluctuation trend becomes more evident with the feed rate goes up. It was reported that the feed rate has a significant impact on serrated chip formation [37]. Based on the correlation of dis-

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locates density and grain size, low-level dislocation density is matched with large grain size, as reflected in Fig. 5(b). The grain size reduces from about 335 to 320 nm with feed rate increasing. Along path 2 from the machined surface into the subsurface, the dislocation density gradually decreases until reaches the initial status. The smaller the feed rate, the quickly declines the dislocation density. When the feed rate is relatively small, the input energy to the machined surface transformed from mechanical energy reduces as well. As a result, the possible dislocation density accumulation induced by a high level of strain or strain rate in the subsurface can be alleviated accordingly. In other words, the storage of the system energy for the full development of dislocation tangles and walls decreases [15]. Similarly, the predicted grain sizes within the subsurface less than 2 µm are nearly the same. With the depth goes deeper, the visibly significant difference in grain size is prominent. The distribution of grain size respectively reaches the initial value at the depth of approximately 20, 35 and 50 µm corresponding to feed rate 0.1, 0.2 and 0.3 mm/rev.

3.1.3. Effect of radial depth of cut

Fig. 6 shows the contour maps of predicted dislocation density and grain size under the various radial depth of cut. The detailed comparison along designated paths 1 and 2 is illustrated in Fig. 7. On the machined surface (path 1), a visible increase in dislocation density to $1.2 \times 10^6$ mm$^{-2}$ is observed when the depth of cut $a_c = 3.0$ mm while insignificant variation is presented between $a_c = 1.0$ and 2.0 mm. It seems that the depth of cut shows marginally influence on dislocation density propagation on the machined surface. Accordingly, the grain size on the machined surface corresponding to $a_c = 3.0$ mm is the smallest about 310 nm with highlighted periodical fluctua-
tion in a wavy shape. Comparatively, the grain size is relatively smaller about 330 nm at a small depth of cut without showing regularly periodical variation. From the machined surface to the subsurface, the variation trend of dislocation density almost overlaps with each other when \( a_{e} = 1.0 \) and 2.0 mm. The accumulated dislocation density along path 2 at depth of cut 3.0 mm is a little higher than the smaller depth of cut. In terms of grain size, there is a marginal difference when the depth of subsurface limited to about 8 \( \mu \)m. The finding is in an agreement with the conclusions reported in Ref. [38]. Once the depth surpasses this magnitude, the grain size affected by the depth of cut is progressively highlighted. In general, the microstructure within subsurface often demonstrates severe plastic deformation or grain distortion [39]. The grain size decreases while the affected depth increases with increasing depth of cut.

3.2. Correlation of serrated segment formation with dislocation density and grain size

As shown in Section 3.1, the suddenly increased dislocation density and reduced grain size along the machined surface (path 1) are particularly highlighted while demonstrating certain periodical regularity. In order to explore and clarify whether this phenomenon is correlated with the formation of the serrated chip, one exemplary case applying the maximum cutting speed during hard milling was provided for investigation. Fig. 8 shows the contour map of predicted dislocation density and grain size. It is apparent that the distribution of dislocation density and grain size in the subsurface present periodical fluctuation in a wavy shape is marked by line 1. More in detail, the variation trend both including dislocation density and grain size in quantitative along paths A and B is illustrated in Fig. 9. Much clearly, the simulated dislocation density and grain size in the subsurface changes periodically in the opposite direction. With the dislocation density accumulation, the corresponding area is inclined to generate dislocation cell or subgrain which defined as grain refinement in this research. Therefore, the grain size variation trend is opposite to the change of dislocation density. In the meantime, the average distance between two peaks is estimated to be 71.75 \( \mu \)m, as plotted in Fig. 9(a) and (b). With respect to dislocation density and grain size alteration along path A in the serrated chip, periodical fluctuation also exhibits with an average distance between two serrated chip segments around 66.37 \( \mu \)m, which shows the intimate relationship exists between the serrated chip formation and the periodical alteration of dislocation density and grain size. On one hand, previous reports have revealed the cutting force fluctuation induced by serrated chip formation [40,41]. On the other hand, the generated chip is unavoidably subjected to complicated behavior like compression, curl and severe friction when flowing upwards. Consequently, it is reasonably speculated that the periodical fluctuation of dislocation density and grain size in the subsurface is the result of serrated chip segment formation during hard milling. Due to the inherent correlation of mechanical property and microstructure, the inhomogeneous distribution of grain size on the machined surface stands a good chance of affecting the functional performance of the machined components.
3.3. Model verification for grain refinement

Fig. 10 shows the mapping relationship between dislocation density distribution and shear deformation zone. Good consistency of morphology between the simulated dislocation density distribution and experimentally observed shear deformation zone is clearly presented including shear band, individual segmentation and machined surface. In other words, the severe plastic deformation corresponds to the propagation and accumulation of dislocation density.

The predicted grain size using dislocation density-based subroutine was compared with the experimentally observed results using TEM. The depth of the subsurface layer for eventually microstructure observation is less than 50 nm after FIB milling. Fig. 11(a) shows the initial tempered martensite lath unit with length around several microns and width around hundreds of nanometers. The dense dislocation is in absence of the bulk material prior to machining. Besides, the corresponding selected area electron diffraction pattern (SAED) for bulk material within the image consists of scattered bright spots indicating the metal crystals in large sizes. In Fig. 11(b), the observed high dislocation density areas are less with a small coverage. In contrast, the appearance frequency of accumulated high dislocation density area is comparatively higher when applying aggressive cutting parameters as shown in Fig. 11(c) and (d). The observed higher density of dislocation in the machined surface is strongly determined by the high strain or high strain rate only achieved by applying aggressive cutting conditions. Although it is unlikely to provide dislocation density assessment precisely through TEM characterization, the bright field transmission micrographs still can offer qualitatively comparison. As indicated by the
Fig. 7 – Dislocation density (a, c) and grain size evolution (b, d) along (a–b) path 1 and (c–d) path 2 ($v_c = 300 \text{ m/min}$, $f_z = 0.2 \text{ mm/rev}$, $a_p = 2.0 \text{ mm}$).

Fig. 8 – Contour maps of (a) dislocation density and (b) grain size ($v_c = 400 \text{ m/min}$, $f_z = 0.2 \text{ mm/rev}$, $a_e = 2.0 \text{ mm}$, $a_p = 2.0 \text{ mm}$).

yellow circle, highly dense dislocation with increasing cover area appears on the machined surface when adopting large cutting parameters. With respect to the simulated dislocation density on the machined surface, it increases from a low level around $1.0 \times 10^{9} \text{ mm}^{-2}$ to a comparatively high level around $1.2 \times 10^{9} \text{ mm}^{-2}$. Strictly speaking, the severe shear plastic deformation during hard milling gives rise to the concentrated dislocation density. Therefore, the TEM results provide reliable proof of predicting dislocation density evolution using the adapted material model.

Fig. 11(b and c) demonstrates the bright field images as well as corresponding SAED under three different cutting conditions. Among the three cutting conditions, it is common to note that the machined surface layer is composed of large
amounts of substructure or dislocation cellular structure without any trace of rod-like lath martensite. With reference to the scale, the sub-grain or dislocation cellular structure size is roughly estimated to be varied in the range of 200–400 nm without much difference among them. In comparison, the SAED spectrum within each micro-graph for surface layer after milling consists of brightly continuous rings, which comprises numerous discrete spots. It is solid proof that a large number of refined crystals usually in nano-scale exist interior the machined surface layer. As discussed simulation results above, the surface grain sizes with subsurface depth in a few microns under various cutting conditions are very close to each other about 320 nm. Consequently, it can be speculated that the subgrain or dislocation cellular structure formed within the machined surface layer is the result of dislocation motion and interaction induced by hard milling. With regard to surface grain size, the predicted results are in good agreement with experimental results. Through analyzing TEM results, the formation procedures of subgrain or dislocation cells in the machined surface layer are illustrated in Fig. 12. At stage I, the rod-like tempered lath units distributed randomly interior the bulk material. At stage II, the lath units are subjected to severe shear deformation along cutting direction leading to the rotation and elongation of lath units in the machining-affected depth. Due to the externally imposed mechanical load, dislocation begins to accumulate and inter-tangle within the lath units during stage III. At stage IV, the inter-tangled dislocation progressively rearranged and form a dislocation wall and eventually results in the formation of subgrain or dislocation cell. Different from microstructure evolution under

![Fig. 9](image_url) Distribution of dislocation density (a, c) and grain size (b, d) along the designated path (a, b) machined surface and (c, d) serrated chip (υc = 400 m/min, fz = 0.2 mm/rev, ae = 2.0 mm, ap = 2.0 mm).

![Fig. 10](image_url) Mapping the relationship between dislocation density distribution and shear deformation zone (υc = 300 m/min, fz = 0.2 mm/rev, ae = ap = 2.0 mm).
4. Conclusions

In this research, grain refinement in the machined subsurface of H13 steel was simulated using a developed multi-physics material model as a result of dislocation density evolution.

Experimental microstructure observation is applied to verify the developed model. Main conclusions are obtained as follows:

(1) A multi-physics model, based on dislocation density alteration, has been adapted applying to predict the grain size evolution in the machined subsurface during hard milling of H13 steel.

(2) With the increase of cutting speed, feed rate and radial depth of cut, grain size on the top-most machined surface vary a little around 330 nm, while gradually increases in the subsurface until it reaches the original size 20 μm with affected depth varies in the range of 25–45 μm.

(3) The periodical fluctuation of grain size in the subsurface is supposed to be induced by the generated serrated chip segments.

(4) With respect to grain size, the observed subgrains or dislocation cellular structure in the range of 200–400 nm matches well with a predicted grain size of about 330 nm. Dislocation density qualitatively also shows a similar variation trend with simulated dislocation density.

(5) The formation mechanism of cell structure/dislocation cell (grain refinement) resulted from the high strain and strain rate is proposed for machining H13 steel with a martensite structure.

As an extension of this work, the material model fundamentally explains the grain refinement mechanism induced by machining from the physical level. While the material-related parameters presented in the theoretical equations also pose a great challenge to obtain accurate simulation results.
Conflicts of interest

None.

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