Micromechanisms and modelling of crack initiation and growth in tool steels: role of primary carbides

Dedicated to Professor Dr. Otmar Vähringer on the occasion of his 65th birthday

Micromechanisms of damage initiation and crack growth in high speed and cold work steels are investigated using scanning electron microscopy in situ experiments. The role of primary carbides in initiation and growth of cracks in tool steels is clarified. It is shown that initial microcracks in the steels are formed in primary carbides and then join together. A hierarchical finite element model of damage initiation, which included a macroscopic model of the deformation of the specimen under real experimental conditions and a mesomechanical model of damage in real microstructures of steels, was developed. Using the hierarchical model, the conditions of local failure in the steels have been obtained. In order to study the effect of carbide arrangement on fracture, numerical simulations of fracture in steels with different ideal carbide arrangements were carried out and compared with each other. It is found that the heterogeneous arrangements of primary carbides can lead to strong deviations of a crack from the mode I path and, therefore, to a significant increase of the fracture energy of the steels.

Keywords: Mesomechanics; Finite elements; Fracture; Damage; Tool steels

1. Introduction

The improvement of service properties of tool steels presents an important source of increasing the efficiency of metalworking industry. In order to develop a numerical model of damage or fracture in the steel, which should serve to predict the lifetime, or to improve the properties, one needs to know the mechanisms of damage and fracture in the steels [1-4].

The direct in situ observation of the fracture mechanisms of the steels under a microscope is quite difficult as compared with the case of more ductile materials, since the material fails abruptly. Then, not only qualitative parameters of fracture (like its mechanisms) but also quantitative ones (like critical damage parameters) are of interest.

The purpose of this work was to study the mechanisms and conditions of damage initiation and growth in the tool steels both qualitatively and quantitatively. The work includes the following steps:

• Scanning electron microscopy (SEM) in situ experiments on 3-point bending of specimens with inclined notches.
• Finite element (FE) simulation of the deformation of the specimens on macro- and mesolevel, taking into account the real microstructure of the steels observed in the SEM -experiments.
• Numerical analysis of the effect of the arrangement of primary carbides in the tool steels on the fracture behavior.

2. Micromechanisms of damage initiation in tool steels

The mechanisms of local failure and critical values for failure of the constituents of the steel have been determined. The constitutive law and elastic constants of the steel con-
In order to clarify the mechanisms of damage initiation and growth in the steels, a series of SEM in situ experiments was carried out. 3-point bending specimens with an inclined notch, as described in [5], were used in these tests. These specimens allow to observe the micro- and mesoprocesses of local deformation and failure of carbides and the matrix of steels during loading of macroscopic specimens in the SEM. The shape of the specimens is shown schematically in Fig. 1a. A photograph of the specimen under loading is given in Fig. 1b. The advantage of the specimen with the inclined notch is that the most probable location of first microcrack initiation in the specimen notch can be simply predicted (which is not the case in the conventional 3-point bending specimens). Therefore, one can observe this location with high magnification during loading and identify exactly the load and the point in time at which the first microcracks form.

Specimens made from the cold work steel X155CrVMo12-1 (in further text denoted as KA) and the high speed steel HS6-5-2 (denoted as HS) have been used. In the experiments, the specimens with different orientations of primary carbide layers were studied. Since the tool steels are produced in the form of round samples and because they were subject to hot reduction after austenitization and quenching, they are anisotropic: the carbide layers are oriented typically along the axis of the cylinder (this is the direction of hot reduction). Therefore, the following designation of the specimen orientation was used: L – the direction along the carbide layers, R – radial direction in the workpiece, C – the direction along the workpiece axis. In the experiments, specimens with orientations CL (the specimen is oriented along the carbide layers; the observed area is oriented along to the ingot axis), LC (the specimen is oriented along the round ingot axis) and CR (the specimen is oriented along the carbide layers; the observed area is oriented normally to the ingot axis) have been used. The specimens have been subjected to the heat treatment (hardening at 1070 °C in vacuum and tempering 2 h at 510 °C), and then polished with the use of the diamond pastes till the roughness $R_z$ of the surface of the specimens does not exceed 3 μm. The notch region of the specimens was etched with 3 and 10 % HNO₃ until the carbides were clearly seen on the surface.

The force-displacement curves were recorded during the tests. The loading was carried out in small steps, with a rate of loading of about 1 mm/s. The places in the specimen notch where microcrack initiation was expected have been observed through SEM during the tests. It was observed that the first microcracks formed only in the primary carbides, and not in the "matrix" of the steel. Also, no microcrack along the carbide/matrix interface was observed in the tests. The forces at which the failure of primary carbides was observed in each specimen are given in Table 1. Fig. 2 shows SEM micrographs of a typical primary carbide in the notch region of steels before and after failure. Since the picture were taken frontal and the specimens used were with the inclined notch, the magnifications of micrographs in x- and y-directions in Fig. 2 are different. In some carbides, multiple cracking was observed as well (see Fig. 3).

Table 1. Critical forces in the tests.

<table>
<thead>
<tr>
<th>Type of the specimen</th>
<th>Force at which a first microcrack was observed in the specimen (N)</th>
<th>Force at which the specimen failed (N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>KALC</td>
<td>95,52,37,5</td>
<td>155,85,160</td>
</tr>
<tr>
<td>KACR</td>
<td>50,55,37,5</td>
<td>95,95,70</td>
</tr>
<tr>
<td>HSCR</td>
<td>45,50,50</td>
<td>95,80,95</td>
</tr>
<tr>
<td>HSLC</td>
<td>50,72,52,127</td>
<td>200,190,195</td>
</tr>
</tbody>
</table>

Fig. 1. 3-point bending specimen: (a) scheme and (b) side view of loading device.

Fig. 2. Carbide grains before (a, c) and after failure (b, d).
Generally, the course of failure of the specimens was as follows:

1. Formation of a microcrack at some carbide.
2. Formation of several microcracks at many carbides at different locations of the observed area (in so doing, the microcracks are formed rather at larger carbides at some distance from the boundary of the specimen, than in more strained macroscopically areas in the vicinity of the lower boundary of the specimen; the local fluctuations of stresses caused by the carbides have evidently much more influence on microcracking than the macroscopic stress field).
3. After the failure of many carbides, the microcracks (or plastic zones in front of the microcracks) begin to grow into the matrix; just after this occurs, the specimens fail. The failure of many carbides was observed just before the specimens failed. Fig. 4 shows a segment of the loaded area with many failed carbides.

3. Condition of failure of primary carbides in tool steels

To simulate the deformation of 3-point bending specimens with inclined notch, a three-dimensional (3D) FE model of the specimen was developed. The forces measured in the tests described above were applied in the simulations. The displacements from the boundary nodes of elements which are located in the vicinity of the symmetry plane and at the lower notch boundary (Fig. 1) are used as boundary conditions in the micromechanical simulation of carbide failure.

Then, the two-dimensional (2D) micromechanical simulations of carbide failure have been carried out for each microstructure and each load, measured in the experiments: a 2D model was created, which represents the cut-out at the notch region of the specimen. The real structure region of the micromodel contains 5000 elements of the plane strain type TRIP 6 and size 100 \( \mu \text{m} \times 100 \mu \text{m} \) and is placed in the lower left corner of the macroscopic 3-point bending model, where the carbide was observed experimentally. As boundary conditions the displacements from the model of deformation of 3-point bending specimen were taken. Since the mesh density in the 2D case is higher, the calculated displacements have been linearly interpolated between the points which were available in the 3D simulation. The micromechanical simulation was performed with the use of the multiphase element method [8–11]. The micrograph of the carbide, obtained in SEM \textit{in situ} experiments was digitized and then automatically imposed on the region of the real structure. The micrographs to be digitized were chosen in such a way that they were representative enough for the given materials. Due to the inclined notch surface, the micrographs in Fig. 2 have different scales in \( x \)– and \( y \)-directions. To take that into account, the micrographs were scaled with the use of the image analysis software XView accordingly to their scales in both directions. The properties of carbide and matrix are as follows [3–6]: (cold work steel) Young’s modulus \( E_C = 276 \text{ GPa} \), \( E_M = 232 \text{ GPa} \), constitutive law of the matrix: \( \sigma_y = 1195 + 1390 \left[ 1 - \exp \left( -\frac{\epsilon_{pl}}{0.0099} \right) \right] \); (high speed steels) \( E_C = 286 \text{ GPa} \), \( E_M = 231 \text{ GPa} \), constitutive law of the matrix: \( \sigma_y = 1500 + 471 \left[ 1 - \exp \left( -\frac{\epsilon_{pl}}{0.0073} \right) \right] \), Poisson’s ratio – 0.19 (carbides) and 0.3 (matrix).
Fig. 5 gives the distribution of von Mises stress in the real microstructure of the cold work steel at the loads at which the carbide failed. Supposing that failure of the carbides is determined by the action of maximal normal stresses, one obtains the failure stresses of carbides for different steels and orientations (see Table 2).

The initial microcracks in the steels are formed within primary carbides (i.e., not along the carbide/matrix interface and not in the matrix). For our further simulation, this means that we can use the multiphase element method. The main input data for the simulation (i.e., the carbide failure condition) was determined with the use of the combined SEM in situ and FE model approach.

### 4. Effect of the arrangement of primary carbides on the fracture resistance of tool steels

As a result of the analysis above, we know the mechanical properties of the constituents of the steel. Then, we seek to study the effect of the arrangement of the primary carbides in tool steels on the fracture behavior of the steels. To do this, we carry out a series of finite element simulations of crack propagation in tool steels with the mechanical properties determined above. Different arrangements of the primary carbides are designed using graphics software, and included into mesomechanical FE models (with carbides as “black” regions and “matrix” as white area). In the simulations, two approaches were used both to take into account the microstructure and to simulate the crack propagation: multiphase finite elements (with “fuzzy” interface between carbides and matrix) for “simple” microstructures, see Figs. 6a–d) and traditional single-phase elements (the interface corresponds to the boundaries of the bodies of FE model and to the element boundaries) for “complex” microstructures, (see Figs. 6e–f), as well as the element elimination and softening techniques. As demonstrated in [10], the methods are fully compatible and give the same results with respect to the crack path, fracture energy and crack roughness, when applied in equivalent cases.

![Fig. 5](image)

**Table 2. Calculated failure stresses of primary carbides in tool steels.**

<table>
<thead>
<tr>
<th>Type of the steel</th>
<th>KALC</th>
<th>KACR</th>
<th>HSCR</th>
<th>HSCL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure stress of carbides (MPa)</td>
<td>1826</td>
<td>1840</td>
<td>1604</td>
<td>2520</td>
</tr>
</tbody>
</table>

![Fig. 6](image)

**Fig. 6. Arrangements of primary carbides in designed “simple” (a–d) and “complex” (e–h) microstructures: (a) band-like, (b) random, (c) net-like, large grains, (d) net-like, small grains, (e–g) layered, (h) clustered. Three orientations of the layered structure are considered: (a) small-large (or S>L) orientation, (f) large/small (or L>S) orientation, and (g) large-small (or L>S) orientation.**

![Fig. 7](image)

**Fig. 7.**

As criteria for the element elimination, the critical values of failure stress (for carbides) and plastic strain (for matrix) were used. The criterion of element elimination in the matrix was determined on the basis of available knowledge about the micromechanisms of fracture of steel matrix. Any damage criteria based on void growth seemed inapplicable in this case due to the mainly brittle macro-behaviour of the matrix. Yet, during SEM in situ experiments, some plastic deformation has been observed at the microlevel (which, however, is quickly followed by the failure of specimens). Thus, we chose the critical plastic strain as a criterion of the element elimination in the matrix. As follows from the SEM in situ experiments described above, the critical plastic strain in the matrix of the steels should be very low. The critical plastic strain value was determined with the use of the numerical experiment technique [8, 10]. At the level of critical plastic strain $e_{phc}=0.1\%$, the small crack increment in the matrix is followed by failure of a carbide in the vicinity of the crack tip, as observed, while e.g. for $e_{phc}=0.05\%$ delayed crack growth occurs.

The following arrangements of carbides were considered: random, net-like (typical for the as-cast state), band-like (typical for the hot formed steels), layered (one half of the microstructure area is filled with randomly distributed small carbides and another half is filled with large carbides) and clustered arrangements (see Fig. 6). In the cases of net-like, band-like, clustered and random arrangements, two types of each microstructure were taken: a fine one with carbide size of 2.5 μm (200 carbides in the area) and a coarse one with carbide size of 3.6 μm (100 carbides in the area). In the case of layered arrangement of carbides, both small and large carbides were combined in one and the same microstructure. The surface area content (in this case, volume content) of the primary carbides was taken to be 10%. Three types of layered arrangements were considered in the simulations, which differ by their orientation relative to the assumed mode-I crack path: (1) Large-small case (or L>S) – a crack propagates first through the part with large carbides, goes through the “interface” (perpendicular to the “interface”) and propagates further through the part...
with small carbides, (2) reverse case (S>L): first, small particle area, then large particle area, and (3) mode-I crack propagates along the “interface” (L/S). For all the simulations, the force-displacement curves were determined numerically. Table 3 gives the nominal specific energy G of the formation of a unit of new surface for the different arrangements of the primary carbides. This value characterizes the fracture resistance of each of the structures, and was calculated on the basis of the force-displacement curves as follows: 

\[ G = \sum_{i} \left( \frac{P_i \mu_i}{L_{RS}} \right) \]

where \( P_i \) is the force for each loading step, \( \mu_i \) is the displacement for each loading step, and \( L_{RS} \) is the size of the real microstructure area (100 \( \mu \text{m} \)). The summation is carried out for all loading steps until the crack passes the real microstructure [10]. Fig. 8 gives two examples of the simulated crack path: a curved/zigzagged, highly energy-consuming crack path in the net-like arrangement of small carbides, and a straightforward, low energy consuming crack path in the band-like microstructure. As parameters of the deviations from the mode-I crack path, we considered the maximum height of the roughness peak \( R_{\text{max}} \). \( R_{\text{max}} \) was calculated from the crack profile as the distance between highest and lowest points of the crack path measured perpendicularly to the initial crack direction (horizontal) [13]. Table 3 gives the values of \( R_{\text{max}} \) for the considered ideal microstructures.

It can be seen from Table 3 that the microstructures which lead to the strong crack deviations (i.e., higher \( R_{\text{max}} \)) ensure rather high fracture resistance. The strong crack path deviations from its initial direction increase the real crack length (i.e., energy consumption in fracture) without increasing the stress intensity factor \( K_I \) [13–14]. One may note that more complex microstructures (like clustered or layered) ensure always higher fracture resistance than the simple symmetric microstructures. The one exception to this rule is the net-like fine microstructure, which forces the crack to follow the carbide network, ensuring the highest fracture resistance, even higher than all the complex microstructures. However, such a mechanism of toughening is unstable: the net-like structure (with larger cells) gives very low fracture toughness; since the crack does not follow the carbide network, but just goes through it.

From the investigations one can conclude that the complex (cluster and gradient) microstructures have a great potential for improving the fracture toughness of tool steels.

5. Conclusions

The mechanisms of damage initiation and growth in tool steels were investigated and the role of primary carbides in damage and fracture of the steels was clarified.

The experimentally observed course of damage evolution in the steels was as follows: One microcrack appears in a carbide, then several microcracks appear in other carbides at different locations of the observed area. In so doing, the microcracks are formed rather at larger carbides at some distance from the boundary of the specimen, than in the macroscopically more strained areas in the vicinity of the...
lower boundary of the specimen. The local fluctuations of stresses caused by the carbides have evidently much more influence on the microcracking than the macroscopic stress field. Finally, after the failure of many carbides, the microcracks (as well as plastic zones in front of the microcracks) begin to grow into the matrix; just after this occurs, the specimens fail. The initial microcracks in the steels are formed in primary carbides (i.e., not along the carbide/matrix interface and not in the matrix). The investigations of the role of the primary carbide arrangements in crack growth allow to draw the conclusions that microstructures which lead to strong deviations from the mode I crack path (for “complex” arrangements of the carbides, like clustered and layered ones) ensure rather high fracture resistances.

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References


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