# MESOMECHANICAL SIMULATION OF CRACK PROPAGATION IN REAL AND QUASI-REAL IDEALIZED MICROSTRUCTURES OF TOOL STEELS

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## *ABSTRACT*

An innovative computational approach to the optimization of fracture resistance of two-phase materials by varying their microstructure is suggested. The main points of the optimization of such materials are as follows: (1) numerical simulation of  crack initiation and growth in real microstructures of materials with the use of multiphase finite elements (MPFE) and the element elimination technique [1-3], (2) simulation of crack growth in idealized quasi-real microstructures (net-like, band-like and random distributions of the primary carbides in the steels), (3) the comparison of fracture resistances of different microstructures and (4) the development of recommendations to the improvement of the fracture toughness of steels. Three main mechanisms of increasing the fracture toughness of steels by varying the carbide distribution (crack deflection by normally oriented carbide layers, crack growth along the carbide network; crack branching) are identified.

## *INTRODUCTION*

The improvement of service properties of tool steels presents an important source of increasing the efficiency of metalworking industry. One of the very promising ways to solve this problem is the computer-aided design of the materials. In this paper, a procedure for the improvement of the fracture

resistance of the steels by the computer-aided optimization of their microstructure (i.e. the distribution of primary carbides, in this case) is developed.

## MECHANICAL PROPERTIES OF STEEL CONSTITUENTS

For the mesomechanical simulation of the deformation, damage and fracture in tool steels, the mechanical properties of the steel constituents are required. The properties of the constituents have been determined experimentally, with the use of microindentation techniques and SEM-in-situ-microbending tests [4, 5]. The properties of the carbide and matrix used in the simulations of the fracture in high speed steel are as follows: $E_C$ = 286 GPa (for M6C carbides) or 351 GPa (for MC carbides), $E_M$ = 231 GPa, $\sigma_F$ = 1604...1840 MPa, where $E_C$ and $E_M$ - Young's moduli of primary carbides and of the matrix of the steel, $\sigma_F$ - failure stress of carbides. The constitutive law of the steel matrix was obtained by CEIT [6] with the means of powder metallurgy, and is as follows (here an approximation is given): $\sigma_y$ = 1500 +1101 [1-exp($-\varepsilon_{pl}$/0.00369)]. The material properties of the high speed steel as a quasi-homogeneous material (such properties are needed for the macroscopic modelling) were taken as follows: Young's modulus E = 236 MPa and Poisson's ratio $\nu$=0.3 [7]. The constitutive law of the steels was [7]: $\sigma_y$ = 2200 + 820 [1-exp($-\varepsilon_{pl}$/0.002)], where $\sigma_y$ – von Mises stress, MPa, $\varepsilon_{pl}$ – plastic strain.

## HIERARCHICAL MODELLING: MACRO-MESO TRANSITION

The crack growth in a real microstructure of high speed steel HS6-5-3 in the short rod specimens is simulated. The diameter of the specimen was taken to be 12 mm, height 18 mm, notch depth 5.32 mm. The simulations were made for 2D plane strain. In the simulations, multiphase finite elements have been used to simulate the real microstructure of the steel, and the element elimination technique to determine the crack path. The displacement of the points in the vertical direction on the plane of symmetry was set to be zero. The point on the symmetry plane of the specimen, which lies on the other end from the notch was fixed in the X-direction as well. The loading was displacement-controlled, and applied in a point at a distance 1.88 mm from the end of the specimen. The loading displacement varied from 0 to 1 mm. The macromodel was constructed in such a way that one could determine the displacement distribution on the boundaries of an area 300 $\mu$m x 500 $\mu$m in the vicinity of the notch. This area presented then the mesomodel, which included also a region with a real microstructure of the steel. The boundary conditions in the mesomodel (the small area 300 x 500 $\mu$m near the notch of short-rod-specimen) were given as vertical displacements. The displacement distribution on the boundaries of the mesomodel was determined from the macromodel, and then approximated by a linear function of loading step in the macromodel and by a linear function of the co-ordinates of a point as $U_y^{micro}$ = f ($N_i$, X), where $N_i$ – the number of the loading step, X – X-co-ordinate of the point of the boundary of the mesomodel. In other words, each loading step in the macromodel, and each point on the boundary of the macromodel have had different values of applied displacements. After approximation, this formula took the form: $U_y^{micro}$ = 0.0002 $N_i$ (-1.96 X +1),

## MESOMECHANICAL MODEL OF CRACK GROWTH IN REAL STRUCTURE

The 2D model with a real microstructure of high speed steel was placed in an area of 100 $\mu$m x 100 $\mu$m near the notch in the mesomodel. As criteria for the element elimination, the critical value of failure stress (for carbides) and plastic strain (for matrix) were used. The critical plastic strain value for the matrix was determined with the use of the numerical experiment technique (this type of modeling is also referred to as inverse modeling) on the basis of the qualitative information about the crack behaviour in high speed steels and the experimentally (in SEM–insitu-tests, see [4,5]) determined carbide failure stress. It is known [8, 9] that a crack in high speed steels is initiated in carbides, if they are available in the vicinity of the notch tip, grows straightforward in the matrix, and kink on the carbide rich regions and

then follows them to a small part, then jumps to the next carbide band, grows in the carbide band furtherly, and so on. We have carried out the simulation of crack initiation with the carbide failure criterion known from [5] and different criteria of crack initiation in the matrix, until the above described crack behaviour was obtained in the simulations. As expected, the most appropriate criteria of the crack initiation in the matrix was the critical plastic strain, and the critical level of this value was $\mathring{a}_{pl} = 0.1$ %. Figure 1 shows the crack growth in the real (band-like) structure of the high speed steel.
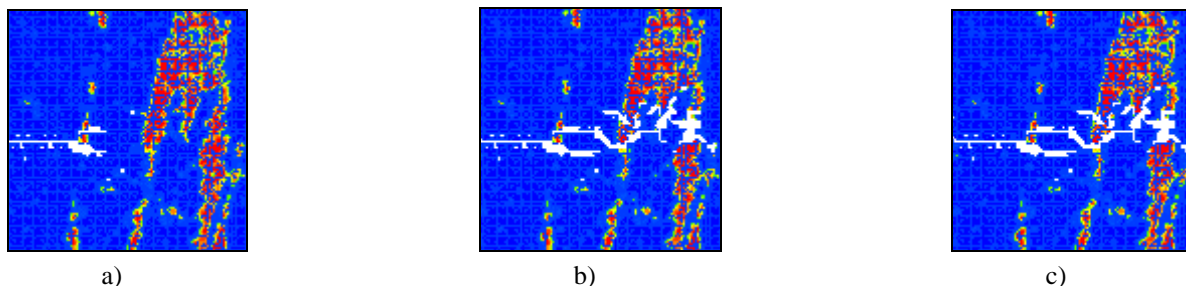


Figure 1. Crack growth in the real microstructure of high speed steel at different displacements u:
(a) u=0.0006 mm; (b) u=0.0008 mm; (c) u=0.0009 mm.

## METHOD OF ARTIFICIAL "REAL" MICROSTRUCTURES

The next step in the numerical optimization of materials is the simulation of deformation and fracture in artificial quasi-real microstructures. By testing some typical idealized microstructures of a considered material in such numerical experiments, one can determine the directions of the material optimization and preferable microstructures of materials under given service conditions. Such simulations should be carried out for the same loading conditions and material, as the real structure simulations which are proved to reflect adequately the material behaviour. Among the types of idealized microstructures, one takes usually as a first approximation the random and periodic microstructures. In studying cast and deformed metals, it is advisable to consider also the net-like (typical for the as-cast state) and band-like microstructures (hot formed steels).
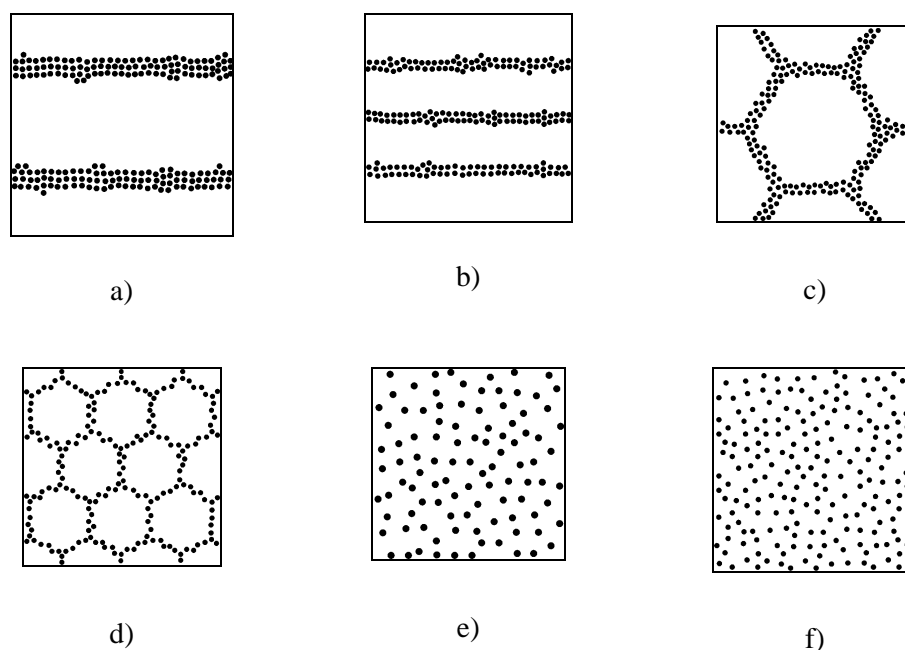


Figure 2. Idealized artificial microstructures of the steel: a) band-like coarse, b) band-like fine, c) net-like coarse, d) net-like fine, e) random coarse, and f) random fine microstructures.

To determine the optimal microstructure of the steel for given conditions, we considered band-like, net-like and random microstructures. Two types of each microstructure were taken: a fine (a carbide size is about 2.5 ìm ) and coarse (a carbide size is about 3.6 ìm ) microstructure. Figure 2 gives the considered artificial microstructures.

### *EFFECT OF MICROSTRUCTURE ON FRACTURE OF THE TOOL STEELS*

Figure 3 show the crack path in the artificial microstructures of the steels. On the basis of the simulations, some quantitative characteristics of the crack growth in the different structures were determined: peak load of the force-displacement curve Fmax, nominal specific energy of the formation of unit new surface G, averaged force Fav, fractal dimension of the fracture surface, height of the surface roughness peaks Rmax. The nominal specific energy of the formation of unit new surface for each microstructure was calculated as follows: $G = \bullet_i (P_i u_i)/ L_{RS}$, where $P_i$ – force for each loading step, $u_i$ – displacement for each loading step, $L_{RS}$ - linear size of the real microstructure, the summation is carried out for all loading steps until the crack passes the real microstructure. The maximal height of the roughness peak Rmax was calculated as the distance between highest and lowest points of the crack path measured along the perpendicular to the initial crack direction (horizontal). The calculated parameters are given in the Table 1.

TABLE 1. QUANTITATIVE PARAMETERS OF FRACTURE BEHAVIOUR OF THE ARTIFICIAL STRUCTURES

| Type of the structure | Net-like | | Band-like | | Random | |
|---|---|---|---|---|---|---|
| | coarse | fine | coarse | fine | coarse | fine |
| Fmax, N | 44.9 | 52.3 | 43.8 | 43.6 | 47.0 | 50.2 |
| G, J/m$^2$ | 436.15 | 827.0 | 341.28 | 676.75 | 699.18 | 557.02 |
| Rmax, ìm | 13 | 36 | 24 | 14 | 18 | 12 |

For both net-like and band-like microstructures the fracture resistance of the steels is much higher for the fine than for the coarse versions of the structures. The difference in the structure of crack path for different microstructures of steels is rather clear: whereas a crack grows almost straightforward in the matrix or between carbide layers, it kinks at the carbide layers or even follows the carbide-rich region if this does not require strong deflection of the crack path from its initial direction. A general tendency is that the maximal height of the fracture surface peak is much more for the coarse than for the fine microstructure (this was not observed for the net-like microstructure only since the full change of the mechanism of crack growth occured in our simulation – the crack in the coarse net-like microstructures grew like in the band-like microstructures, i.e. by jumps between carbide layers).

It is of interest that the averaged force Fav hardly increases with increasing the peak load. If one considers only the coarse microstructures, one can see that the Fav even decreases with increasing the peak load Fmax. So, increasing the resistance of the materials to the crack initiation does not mean necessarily the increase of the energy consumption in crack growth (i.e. fracture toughness). This suggests that a gradient microstructure of steel may be optimal in this case: namely, in the parts of the cutting tool, in which the tensile stresses are maximal and the crack initiation is therefore most probable, microstructures which ensure maximum Fmax should be used (first of all, the cutter face, especially in the vicinity of the cutter edge is meant). In the rest of the tool material, a microstructure which ensure the maximum energy consumption in crack propagation should be taken.
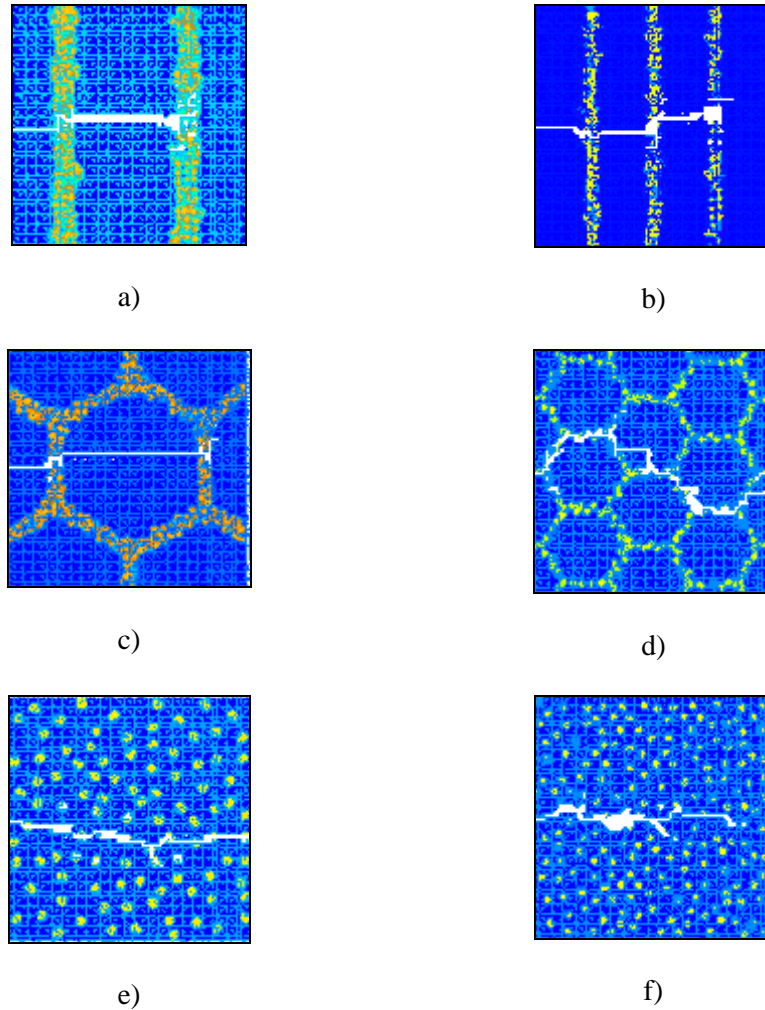
Figure 3. Crack growth in different artificial microstructures: a) band-like coarse, b) band-like fine, c) net-like coarse, d) net-like fine, e) random coarse and f) random fine microstructures. Displacement u= 0.0006 mm

## *FRACTALITY OF FRACTURE SURFACE*

Considering the crack as a cluster from the aggregated eliminated elements, one may determine the fractal dimension by the formula: $i \sim L^D$, where i – the amount of particles (in our case, the amount unit steps of the crack growth, or eliminated finite elements), L – projected crack length. To determine the fractal dimension of the crack path from above simulations, we determined the amount of eliminated elements and the projected length of the crack after each loading step, and determined the power in the i-L-relationship for each of the structures. The fractal dimensions for each microstructure are as follows: net-like microstructure: coarse: 1.285, fine: 1.593; band-like one: coarse: 1.442, fine: 1.40; random microstructure: coarse: 1.372, fine: 1.446. One can see that the maximal fractal dimension is in the band-like fine microstructure. The relationships between the specific fracture energy and the fractal dimension of the fracture surface is shown in Figure 4. One can see that although the results of our numerical experiments (similarly to conventional experiments) show a great dispersion of the results, the tendencies are still rather clear: the specific energy of fracture increases with increasing the fractal dimension of the fracture surface. It is worth to note that the appearance of the curve corresponds to the relationship between the surface energy of fracture and the fractal dimension derived in [10]: $G \sim (a/L)^{1-D}$, where a – yardstick length (this value may be taken to be equal to the carbide size [11]), L – unit length (a value of the order of crack length).
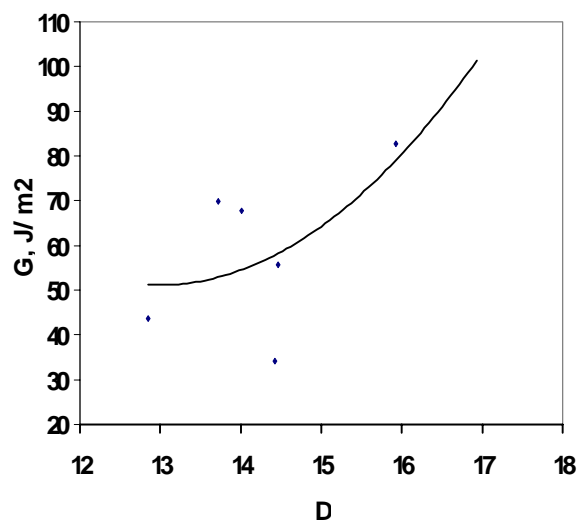
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Figure 4. Specific energy of fracture plotted versus the fractal dimension of fracture surface.

## CONCLUSIONS

The following effects which increase the toughness of the steels were observed in the considered structures: (1) crack deflection by carbide layers oriented perpendicular to the initial crack path (in net-like coarse microstructures, band-like microstructures), (2) the crack follows the carbide network (net-like fine microstructure), and (3) damage formation in random sites of the steels and following crack branching (random microstructures). Whereas all the modes of steel toughening ensure (or tend to ensure) comparable levels of fracture toughness, the type of microstructure (and, therefore, the mode of toughening) for given conditions should be chosen on the basis of the economical considerations of the steel production and other requirements like the wear resistance of the tool, etc.

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