

DESCRIPTION OF MULTIPLE CRACKING IN UV-DEGRADED STRESSED POLYETHYLENE USING PERCOLATION APPROACH

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ABSTRACT

Description of an evolution of damage, spread in bulk of material, remains for the time being a complex problem. The fracture mechanics approach is not capable to deal with the problem in general, since for the large ensembles of defects it requires lot of information and becomes too cumbersome. As a compromise the use of some physical theories, for instance percolation theory, can be suggested. These theories neglect some information related to individual characteristics of defects (in the other words they operate with the parameters of groups of defects).

Percolation theory deals with so-called "disordered systems", predicting behavior and certain properties of these systems, based on the properties of their elements. For simulation of cracking phenomenon, the possibility "to fail" is assumed for arbitrary element of this system. Then, using percolation theory approach, it is possible to study the dependencies between the probability of element' failure and formation of cluster of "failed elements", which connects opposite sides of the system (splitting it apart).

In frames of the traditional percolation theory it is assumed, that the elementary failure events should be independent. However, the damage evolution is affected by the long-scale stress-strain field, which, in turn, depends on the present distribution of damage. Hence, the percolation theory should be adapted to account for the long-scale fields (i.e. correlation of events). In this paper the elements of simulation approach, which includes both: elements of percolation theory and damage mechanics, is outlined. The approach is demonstrated by modeling surface cracking of high-density polyethylene due to it UV-degradation under mechanical loading.

KEYWORDS

Percolation approach, Finite Element analysis, damage evolution, surface cracking, UV-degradation

INTRODUCTION

The fracture mechanics' approach is not capable to describe the multiple cracks, developing quasi-uniformly in the bulk of material. Recently, in order to cope with the problem the percolation approach is employed [1 – 7] more and more intensively. The main attention here is paid to the process of formation of crack'

networks, connectivity of such networks and also to parameters, which can characterize these structures, like: percolation threshold, correlation radii [8] or excluded volume [7].

Although these studies have been performed on different geometrical objects (discrete and continuous) and have had different subjects (i.e. parameters) to be investigated, there are some features that are common for these studies. The “elementary failure events” have been assumed to be independent: in the other words, in all the cited papers only geometrical aspects of the crack’ networks have been studied. In reality, however, the cracks grow, while affected by the long-scale stress field as well as by the other cracks. In order to account for this feature of the crack’ networks evolution, the percolation theory approach should be modified. In this paper the elements of simulation approach, which includes elements of both: percolation theory as well as damage mechanics, is outlined. The approach is demonstrated for the case of modeling of surface cracking of High-Density Polyethylene (HDPE), degraded under UV-radiation and mechanical loading.

MAIN ELEMENTS OF PERCOLATION SIMUALTION APPROACH

Percolation theory [8] is an interdisciplinary field of research that constitutes mathematical method for the theory of critical phenomena and phase transitions [9]. It deals with the properties of so-called “disordered systems” (it can be a spatial lattice or a random spatial distribution of geometrical objects), which rise as the collective properties of its elements.

In order to model development of intergranular damage in polycrystalline material, the Voronoi tessellation was chosen as the object for percolation simulations, since the principle of formation of this tessellation is accordant with the principles that constitute the formation of a polycrystalline solid. The “possibility to fail” is assigned to every element in the tessellation. Using random numbers seed an “elementary failure” is drawn for every element. Next, clusters (i.e. sets of connected “failed” elements), their properties and evolution are to be monitored. Further, the lattice is scanned for a “percolated cluster”, which connects two opposite sides of the tessellation, i.e. splits the object studied into two parts. The probability of percolated cluster formation (and corresponding “percolation thresholds”) is to be evaluated.

There are several studies [10 – 12], where the Voronoi tessellation is being considered as the object for percolation studies. All of them, however, consider non-correlated percolation and none of them consider percolation as the model for fracture phenomenon of a polycrystalline solid. The elements of cluster labeling (in the other words: preparation for clusters’ generation) for random lattices is given in [13, 14]. Further we will describe only some elements, related to simulation of correlated percolations. As mentioned above the “elementary failure” events in this model are correlated, but not directly – only through the long-scale field (namely stress-strain field). In order to construct such relation the stress-strain field should be calculated (for instance using Finite Element method) and mapped into the Voronoi tessellation (Fig. 1). Further the results of percolation simulations on the Voronoi tessellation at the end of every increment should be again mapped into Finite Element package. The above exchange of data was arranged in real time regime: in the other words, the Finite Element program and program for percolation simulations were waiting on each other at the moment, when the data from the other program are not yet calculated.

Unlike in the investigations [14, 15], where direct percolation was studied, the decision about “elementary failure occurrence” was derived, based on the completion of deformational criterion:

$$\varepsilon_{crystall} + \varepsilon_{external} = \varepsilon_c, \quad (1)$$

here $\varepsilon_{crystall}$ is a deformation of material due to internal stresses, $\varepsilon_{external}$ denotes external deformation and ε_c means the critical deformation level. The stochastic data concerning the failure of elements of the Voronoi tessellation were transformed to the continuous damage field ω by averaging of the results of percolation simulations over the λ -size regions [15].

This approach was used to study the surface cracking in UV-degraded and mechanically loaded HDPE.

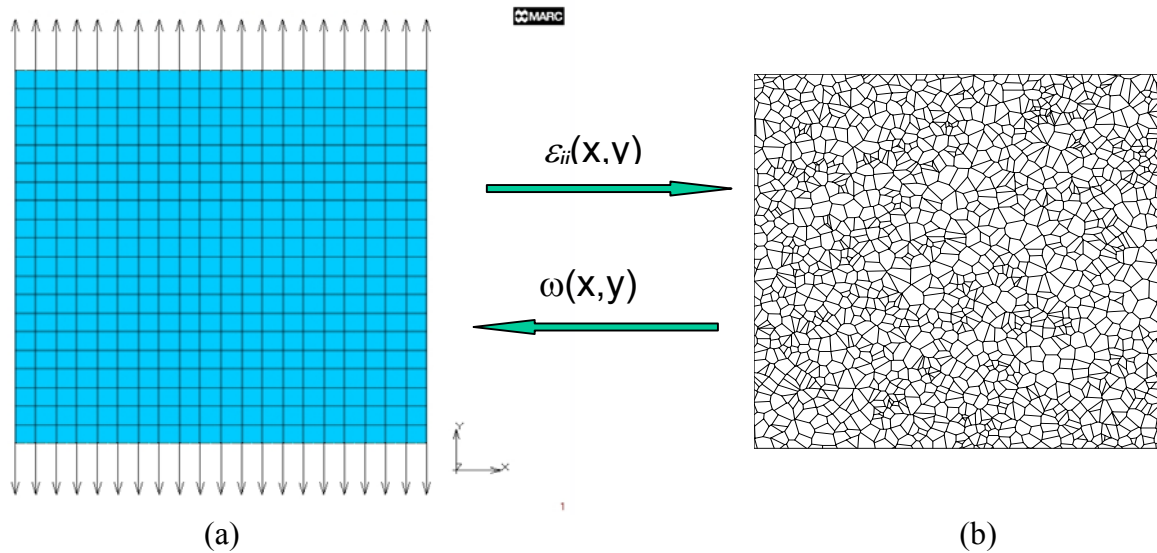


Figure 1. The scheme of data exchange between two parts of simulation process: FE modelling (a) and percolation simulation (b).

SOME ASPECTS OF BEHAVIOUR OF UV-DEGRADED HDPE

The main physico-chemical features of ultra-violet (UV) degradation of HDPE, which relate to surface cracking of material, are given in [14, 15]. Substantial drop in the material ductility with time (fig. 2,a) inevitably leads to the moment, when the critical strains ε_c become lower, than the local strains in polymer. In other words the deformational failure criterion $\varepsilon = \varepsilon_c$ turns out to be locally feasible, what results in the cracking along the crystallites' boundaries. These local strains ε might be the result of either mechanical loading (let us call them “external strains”) or microstructural changes induced by UV-degradation of polymer (“internal strains”). Latter might be resulted by so-called “shrinkage due weathering” [16, 17].

The micromechanism of this phenomenon is as follows. The UV-degradation of polymer leads to additional crystallization of material: i.e. the amorphous regions that are closest to the crystalline lamellas transform into crystalline regions with the time passing by. The example of crystallinity' evolution in 0.2mm HDPE film during UV-degradation test is presented in fig. 2b. Since the density of HDPE crystalline phase ($\rho_c=1.001 \cdot 10^6 \text{ g/m}^3$) is higher, than that of amorphous phase ($\rho_a=0.856 \cdot 10^6 \text{ g/m}^3$) [18], the crystallinity growth leads to rise of total density of degraded material, which can be calculated as follows [19]:

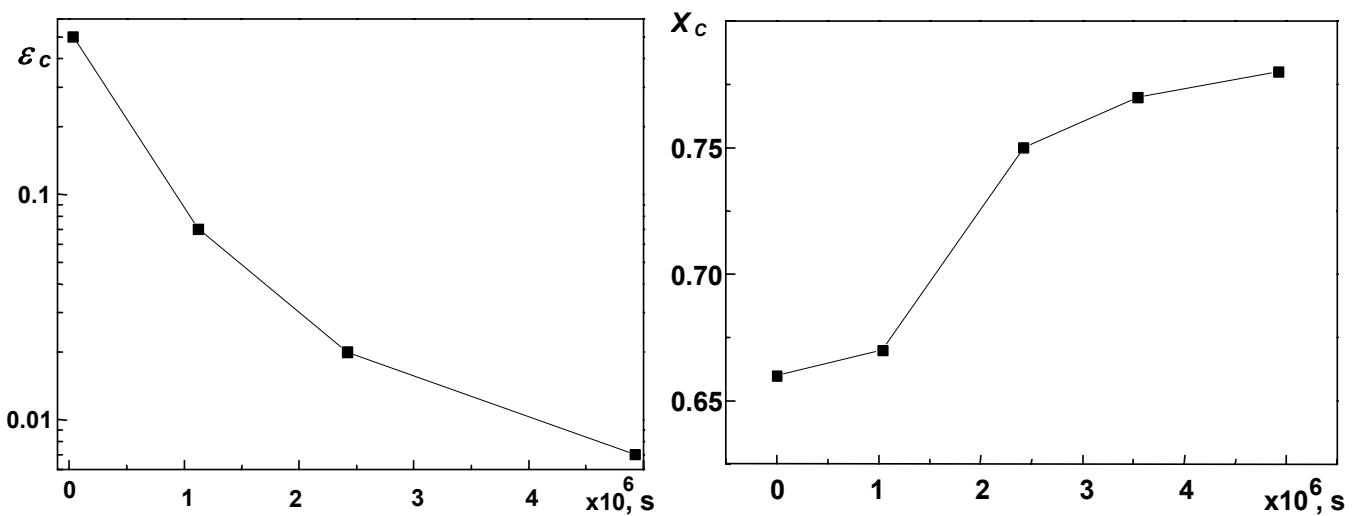


Figure 1. Strain failure, (a) and crystallinity X_c (weight fraction), (b) versus time of exposure to UV-radiation for 0.2mm HDPE film. Strain at failure registered for tension rate $3 \cdot 10^{-6} \text{ s}^{-1}$, [19].

$$\rho_{tot} = \rho_c \rho_a [\rho_a X_c + \rho_c (1 - X_c)]^{-1}. \quad (2)$$

Assuming that the mass growth of polymeric material due to oxidation is small, the increase in density should lead to drop in volume of degraded polymer (i.e. degraded material “shrinks”).

It should be noted that since UV-degradation requires constant replenishment of oxygen in material from surface, the spatial distributions of solved oxygen (as well as of the products of oxidation reactions) are formed [19]. In other words, the near-surface regions in polymers are most subjected to the UV-degradation and, hence, additional crystallization. Since these near-surface layers are tied with the bulk material, which does not suffer from these phenomena, the bulk material prevents these near-surface regions from shrinkage, what certainly will induce straining of outer surfaces:

$$\varepsilon_0(t) = [V_0 - V(t)]/V_0. \quad (3)$$

Here V_0 is the original volume (and the constant volume of bulk material, linked to considered part of surface); $V(t)$ denotes the variation of volume of degraded surface layer due to shrinkage. Taking into account the above assumption about the stability of polymer mass during weathering and, that the volume of a whole part consists of volume of amorphous and crystalline parts, the eqn. (3) can be rewritten as follows:

$$\varepsilon_0(t) = 1 - [(1 - X_c(t))\rho_c + X_c(t)\rho_a] \times [(1 - X_c(0))\rho_c + X_c(0)\rho_a]^{-1}. \quad (4)$$

Based on these phenomenological relations earlier [15] the simulation of surface microcracking in UV-degraded HDPE using percolation approach was performed. That study, however, accounted only for the internal strains as the possible reason for microcracking (i.e. correlation due to the long-scale field was neglected).

For simulation of the evolution of strain' field in UV-degraded HDPE the generalized Schapery model of relaxation type was modified in order to account for a continual damage parameter ω :

$$\varepsilon_{total} = \varepsilon_{ve} + \varepsilon_{pl}; \quad \frac{\partial \varepsilon_{pl}}{\partial t} = C \left(\frac{\sigma - \sigma_0}{1 - \omega} \right)^\lambda; \quad (4)$$

$$\sigma(t) = E_0 g_0(\varepsilon_{ve})(1 - \omega) + \sum_i D_i (1 - \omega) \exp(\beta_i \varepsilon_{ve}) \int_0^t \exp[-\lambda_i (\zeta_i - \zeta'_i)] \frac{\partial [(\varepsilon_{ve})^{\alpha_i}]}{\partial \xi} d\xi; \quad (5)$$

$$\zeta_i(\xi) = \int_0^\xi \frac{d\xi}{a_i(\varepsilon_{ve})}; \quad \zeta'_i(t) = \int_0^t \frac{dt}{a_i(\varepsilon_{ve})}; \quad a_i(\varepsilon_{ve}) = \exp[\gamma_i \varepsilon_{ve}]. \quad (6)$$

The model parameters used for FE simulation of visco-elastic behavior of HDPE are given in Table 1 [20]. The details of the implementation of the model (4) – (6) in FE package MARC [21] are given in [22]. For this the user subroutine HYPELA [23] was employed.

Table 1. The set of model parameters for description of creep-recovery behaviour of HDPE

i	D_i	α_i	β_i	γ_i	λ_i
1	.5976498·10 ³	.1145182·10 ¹	-.259844·10 ²	-	10 ⁺¹
2	.140191·10 ³	.8490412	-.1368976·10 ²	.1786815·10 ¹	1
3	.9025508·10 ³	.132205·10 ¹	-.1379134·10 ²	.9235095	10 ⁻¹
4	.8507839·10 ²	.8708816	-.2221988·10 ²	-	10 ⁻²
5	.1189788·10 ³	.9295784	-.1058856·10 ²	.5253887·10 ¹	10 ⁻³
6	.1578546·10 ³	.9738781	-.494870·10 ²	-	10 ⁻⁴
7	.5585853·10 ²	.9941104	-.1252381·10 ²	.7399315·10 ¹	10 ⁻⁵
8	.6601488·10 ³	.9040428	-.1707527·10 ²	.5363343·10 ¹	10 ⁻⁶
9	.2640200·10 ²	.123677·10 ¹	-.4865952·10 ²	.129430·10 ²	10 ⁻⁷
	D_0	α_0	E_0	C	γ
	.520395·10 ²	.7241752	.1036215·10	.1499238·10 ⁻⁵	.121962·10 ¹
					σ_0
					.9810459·10 ¹

RESULTS OF MODELING

As the example for simulations an HDPE square plate, subjected for uniaxial tension and UV-degradation, is considered (fig. 1). Since the size of the Voronoi tessellation (i.e. number of elements in the tessellation) influences the results of percolation simulation (scaling effect), it is necessary to perform simulation for a set of lattices of different size. Next, using specific extrapolation technique [8], the conclusions concerning the behavior of infinitely large meshes can be derived. In this study the simulation was performed for 4 levels of stresses: 1, 3, 6 and 10 MPa. It was shown that for this model the percolation threshold p_c weakly depends on the stresses level (Table 2).

Table 2. Percolation threshold p_c of UV-induced microcracking in HDPE depending on the stress level

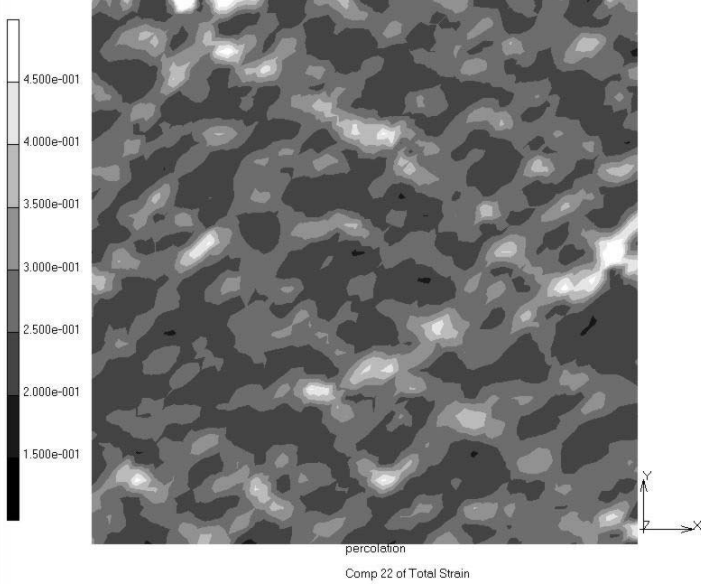
Stress level, MPa	-	1	3	6	10
Percolation threshold p_c	0.6307	0.6363	0.6627	0.6773	0.6821

In the fig. 3 the variation of strain field and distribution of failed elements on the Voronoi tessellations versus stresses, applied to square plate, is given for the final moment of simulation at three stress levels: 10 MPa (Fig. 3, a), 3MPa (Fig. 3, b) and 1MPa (Fig. 3, c). The comparison of these fragments demonstrates an increase of the role of effective strains with the growth of the stress level: with the growth of stresses applied the formed clusters orient along the maximal shear strain direction.

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Inc : 33
Time : 9.300e+005



MARC

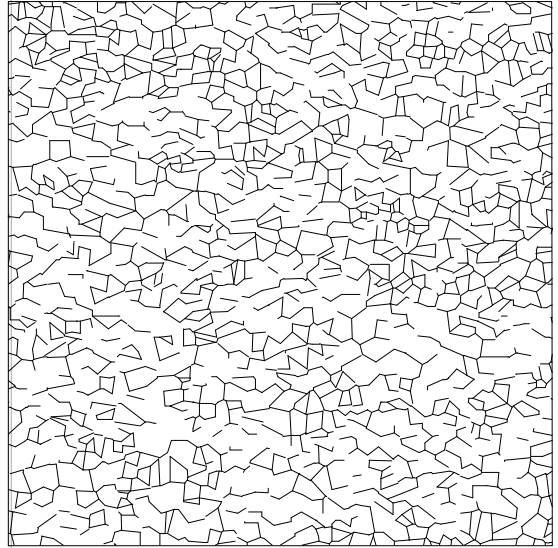
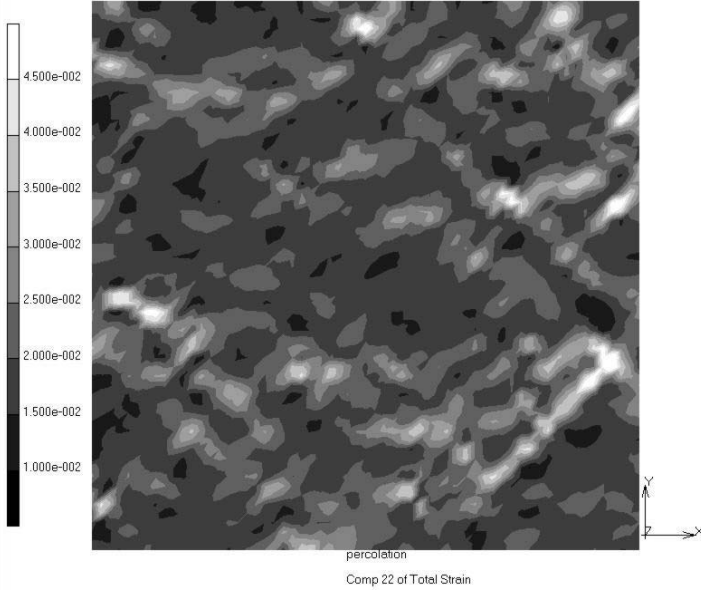


Figure 3, a.

Inc : 39
Time : 3.370e+006



MARC

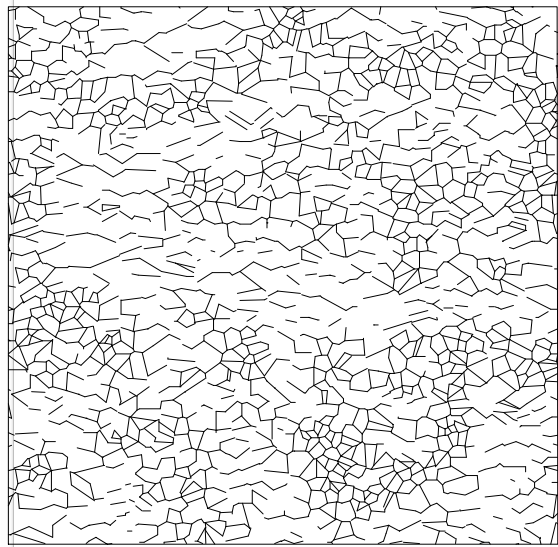
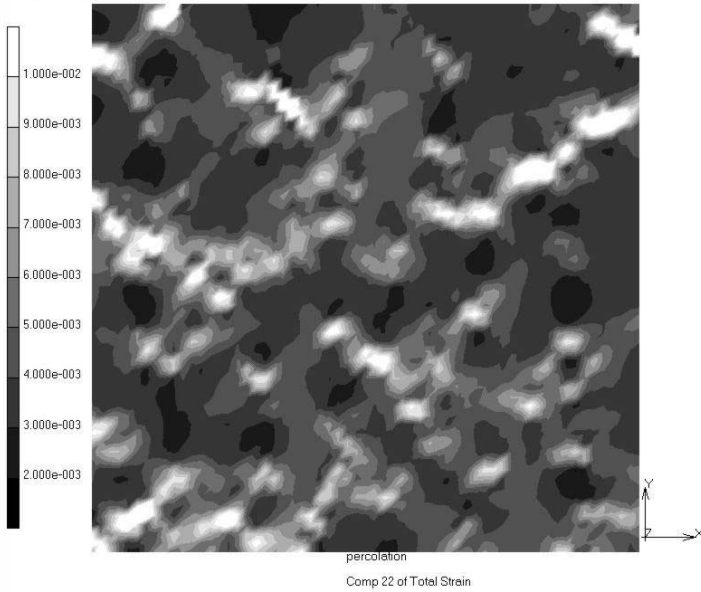


Figure 3, b.

Inc : 37
Time : 3.625e+006



MARC

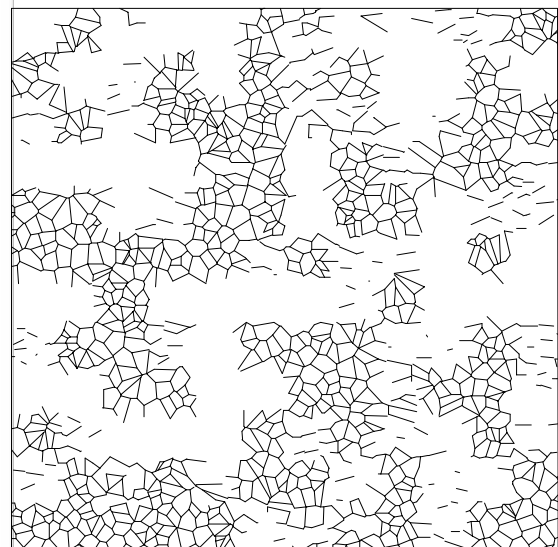


Figure 3, c.