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Characteristics of high-density polyethylene and its properties simulation with use of finite element method

RAPID COMMUNICATION

Summary — It the paper, an analysis of strength characteristics of polyethylene products, obtained by different methods of processing was presented, to obtain definite input data for numerical analysis with the use of finite element method (FEM). The dependence of variations of stress and deformation values on the conditions of tests was analyzed using as examples the samples of high-density polyethylene obtained in the technological processes, subjected to the uniaxial tension at a testing machine. Crystallity degree was determined for the samples obtained from extruded or injected products. The changes of internal characteristics of the products were tested in chosen areas of testing samples under influence of external load increasing in time. The results of laboratory tests formed the basis for development of the characteristics of material and values of parameters for numerical models were determined, dependently on the method applied for polymer sample production. The numerical simulations were conducted in linear formulation, being the simplified analysis in the scope of Hooke's law being in force, and also in physically non-linear range, taking into account the real characteristics of plastic during the process of sample loading. The numerical investigations allowed to define the state of strain and stress in the whole sample analyzed dependently on the processing conditions.

Key words: polyethylene, mechanical properties, crystallinity degree, finite element method analysis.

CHARAKTERYSTYKA POLIETYLENU DUŻEJ GĘSTOŚCI I SYMULACJA JEGO WŁAŚCIWOŚCI METODĄ ELEMENTÓW SKOŃCZONYCH

Streszczenie — W artykule przedstawiono analizę cech wytrzymałościowych wytworów z polietylenu, otrzymanych różnymi metodami przetwórstwa, celem uzyskania określonych danych wejściowych do analizy numerycznej z wykorzystaniem metody elementów skończonych (MES, ang. *finite element method*). Próbki z polietylenu dużej gęstości poddano jednoosiowemu rozciąganiu z wykorzystaniem maszyny wytrzymałościowej i przeanalizowano zmiany wartości naprężenia oraz odkształcenia w zależności od warunków prowadzenia badań. Określono także stopień krystaliczności próbek otrzymanych z wytworu wytłaczanego i wtryskiwanego oraz badano zmiany, pod wpływem narastającego w czasie obciążenia zewnętrznego, cech wewnętrznych wytworu w wybranych obszarach próbek badanych. Na podstawie wyników badań laboratoryjnych opracowano charakterystyki materiałowe i określono wartości parametrów modeli numerycznych, w zależności od zastosowanej metody wytwarzania próbki. Symulacje numeryczne prowadzono w ujęciu liniowym, stanowiącym uproszczoną analizę w zakresie obowiązywania prawa Hooke'a, jak również w zakresie fizycznie nieliniowym, uwzględniającym rzeczywiste charakterystyki tworzywa w trakcie procesu obciążania próbki. Badania numeryczne pozwoliły na określenie stanu odkształcenia oraz naprężenia w całej próbce w zależności od warunków jej wytwarzania.

Słowa kluczowe: polietylen, właściwości mechaniczne, stopień krystaliczności, analiza metodą elementów skończonych.

The design of the new products from polymer plastics requires the knowledge of many mechanical properties of plastics, technological conditions of production and at last, the knowledge of future expectations referred to high by useful parameters. From the point of view of mechanical properties, the factors decisive for value of maximum load are boundary strains and stresses versus time [1—2]. The same product can some-

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times be produced at wide variety of processing conditions within a given method, and show entirely different structures, as well as different external and internal characteristics of the whole product or its precisely chosen area [3, 4]. Many computer programs exist at designers' disposal for simulation of the production process making possible the analysis of conditions of flowing and molding of the product in basic processing processes. These programs *i.e.* Moldflow, Fluent, Extrud and others concern mainly the classical processes of injection molding or extrusion. Programs require some information on basic rheological properties of plastic at variable thermal conditions [5, 6]. The existing methods of determination of the viscosity curve on a basis of the one parameter only — the melt flow rate (*MFR*) coefficient with the use, for example, of Winogradow and Malkin model, are absolutely insufficient in this case [7, 8]. They have too much universal character and do not guarantee the needed precision of a simulation. Therefore, in numerical applications the Bird-Carreau-Yeshuda rheological model is used, and calculations are complemented with additional Arrhenius or Williams-Landel-Ferry equations, dependently on crystallinity degree of polymer [9]. When the adequate equations to calculations are used, the received results of computer simulation give visualisations of phenomena related to the production conditions. However, to obtain the proper product, the required mechanical characteristics and useful properties have to be verified. Another group of simulating programs are these, which are designed for strength analyses making possible to check the correctness of the whole construction operation, its chosen units or whole mechanism operation in preliminary stage. In this case, the calculations are based on discreet models, in which the finite element method (FEM) has the most universally application. The following packets can be included in this type of programs: Catia, Ansys, Nastran, Abaqus and others [10, 11]. Use of the input data describing material only through the basic parameters, such as Young's modulus and the value of Poisson's ratio, is sufficient for metals. However, in the case of polymers, these quantities describe behavior of this type of materials in small degree only. Sometimes, the basic material data are useful at calculations in very small range of changes of external input functions, in the form of linear characteristic of material, and therefore in the range in which Hooke's law is in force. Therefore, determination of characteristics of plastic, from which a construction subjected to real, greater input functions, has to be produced is not a simple task. The large number of industrial branch standards and standard specifications exists [12—15], as well as many forms of machines and measuring devices for determination of the characteristics and chosen properties of plastic parts are used, influencing the studied sample through static or dynamic loads. All results of these tests are connected with a definite method and test stand, and in majority of cases they can not be compared without indication of all detail information.

EXPERIMENTAL

Material

The plastic used to test was high-density polyethylene ($MFR_{(190,5)}$ = 1.25 g/10 min, Poisson's ratio 0.42). Samples for laboratory tests were obtained with the use of extrusion or injection molding methods. The testing specimens were obtained according to the suitable standards [13—15]. The dimensions of specimen cross-section in the middle of its length were respectively 4×10 mm.

Methods of testing

Mechanical properties

Measurements were carried out with use of tensile testing machine of FPZ -100/1 type, class 1.0. The tensile test was conducted at temp. 22 ^{o}C, at three varying values of tensile rate equal to 20, 50 and 80 mm/min. During tests the deformations of specimens were measured (Fig. 1) using a DA extensometer of III 99950-5330 type.

Fig. 1. View of sample during test using tensile testing machine with the use of DA extensometer

Crystallinity degree

Crystallinity degree ($w_{c,h}$) was determined applying calorimetric method. For TGA/DSC investigations an apparatus of Mettler-Toledo was used. Samples *ca.*10 mg were taken and were weighed with accuracy ± 0.001 mg in standard aluminum weighing bottles. The heating was conducted with rate 10 ^{o}C/min. Temperature measurement and thermal calibration were carried out according to guidelines of calorimeter's manufacturer.

Simulating tests in FEM formulation

The subjects of numerical analysis in FEM formulation were models mapping the element of polyethylene material in the form of tensile specimen, being the standardized test sample. The determination of the state of specimen transverse section deformation was the aim of the analysis, as well as the reduced stress distribution determined according to strength hypothesis of Huber-Mises-Hencky (HMH) in an area of numerical model in dependence of applied material model HMH hypothesis was applied for solid body mechanics to determine effort grade. Abaqus/Standard software by SIMULA Dassault Systems was used as numerical tool in calculation [16, 17], which has allowed FEM analysis taking into consideration nonlinear problems. It is especially important for materials properties and large displacement modelling. Two kinds of material models were assumed for samples obtained by extrusion or injection molding methods: linear and non-linear ones. In the case of linear models, the value of Young's modulus was obtained as a result of laboratory tests. In the calculation for non-linear model of material, the multi-linear characteristics of elastic-plastic material was assumed and Newton-Raphson analysis method was used [11]. Model was built on the basis of stress-strain curves obtained in the result of experimental tests, for different deformation rate of the specimens.

RESULTS AND DISCUSSION

As a result of mechanical tests, the values of longitudinal modulus of elasticity were determined, equal to E = 736 MPa for the extruded samples, and E = 637 MPa for the injected ones. The obtained results of changes of stress value in the function of strain for different tensile rates and the remaining parameters constant were presented in Fig. 2.

The investigations of crystallinity degree were targeted at the assessment of differences in structures obtained in two separate technological processes, as well as the changes of structures resulting from the forced load at assumed maximal rate of deformation 80 mm/min. The degree of polymer crystallinity was defined as fractional content of polymer crystalline structural constituent in relation to amorphous mass fraction. The crystalline structured constituent and the amorphous structural constituent in the sample have the same properties as the corresponding ideal state. In the case of applying calorimetric methods crystallinity degree ($w_{c,h}$) were calculated:

$$w_{c,h} = \frac{\Delta h_t}{\Delta h_{t,c}} \quad (1)$$

where: Δh_t — *heat of fusion of the polymer sample*, $\Delta h_{t,c}$ — *heat of fusion of the entirely crystallized polymer.*

The value of thermal effects of polymer melt Δh_t is defined on a basis of DSC curve (presented in Fig. 3) registered during heating of sample with constant rate [18]. Crystallinity degree values obtained for extruded and injected samples are listed in Table 1.

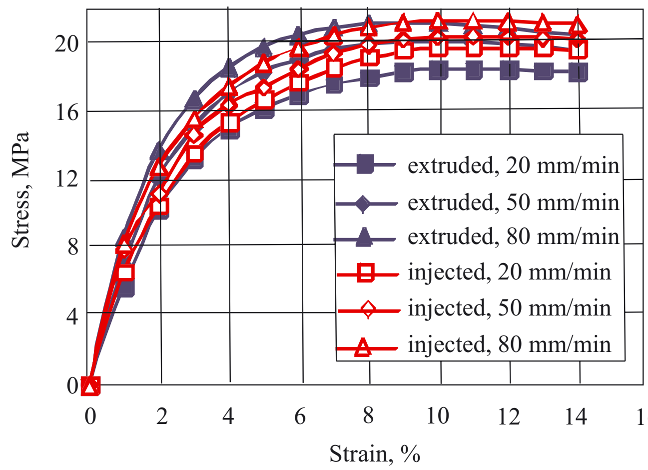

Fig. 2. Stress-strain curves obtained at different rates of test (20, 50 or 80 mm/min) for samples extruded or injected

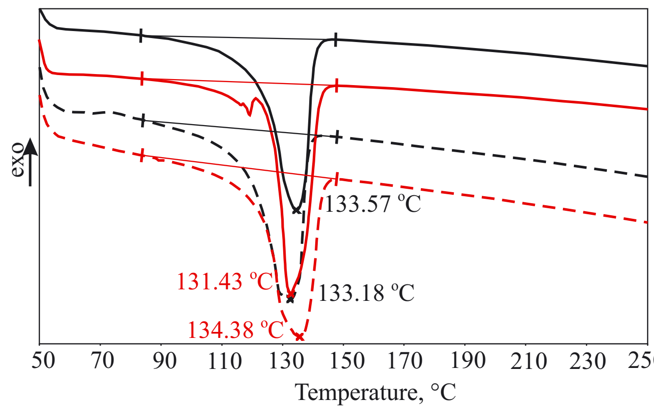

Fig. 3. DSC curves for the samples produced by extrusion (solid lines), or injection molding (dashed lines); black color presents behavior of sample taken from the place in vicinity of fixture of machine, red color corresponds to sample taken from the place of break

Table 1. Crystallinity degree of extruded and injected samples taken from different areas of the specimen (temperature range from 84 °C to 148 °C)

Type of sample/measure place	Mass, g	Temperature peak, °C	Crystallinity %
extruded/main place	$1.119 \cdot 10^{-2}$	133.57	47.24
extruded/narrowing place	$1.090 \cdot 10^{-2}$	131.43	48.50
injected/main place	$0.979 \cdot 10^{-2}$	133.18	50.25
injected/narrowing place	$1.050 \cdot 10^{-2}$	134.38	50.46

The digitization of numerical model of sample was based on eight nodes solid elements, possessing three degree of translation freedom in each node. The structural net of finite elements of the type *hex* was applied

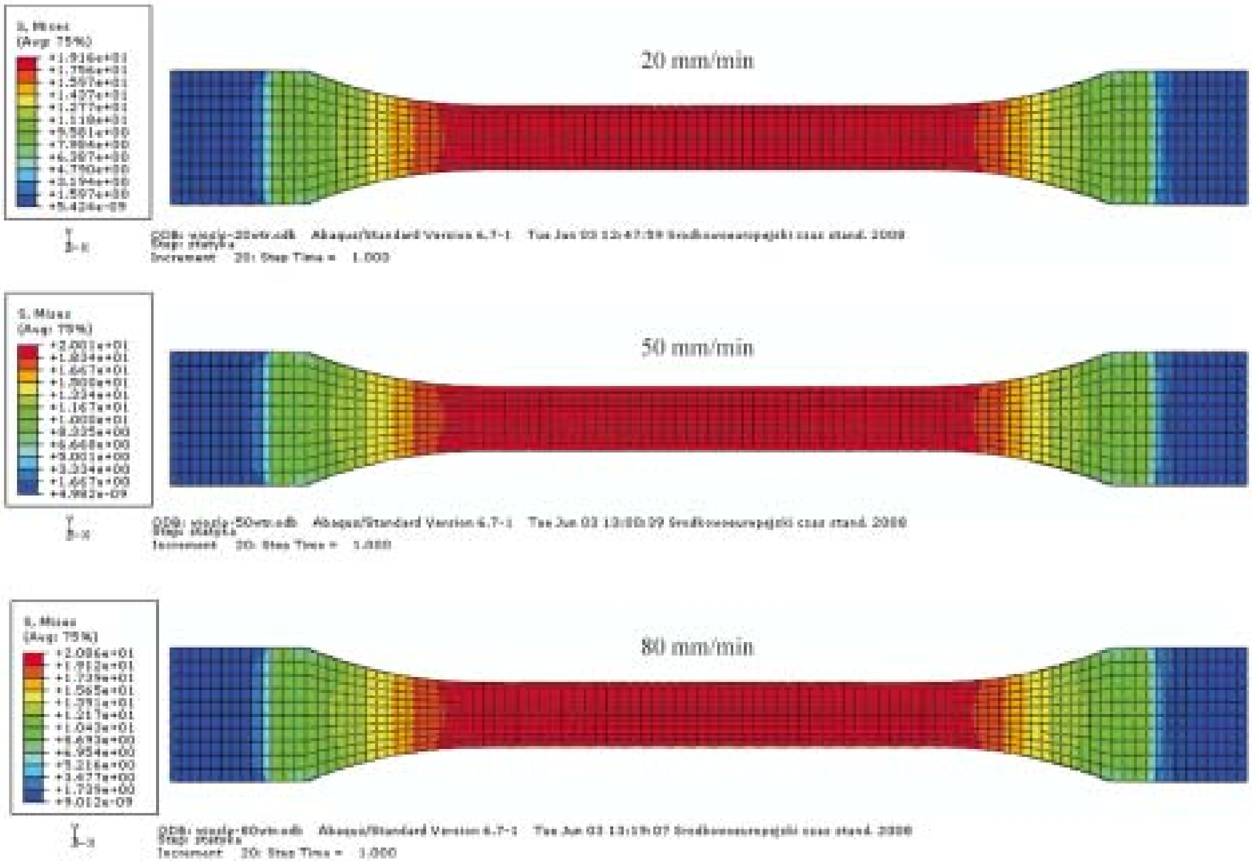

Fig. 4. Example of the results of reduced stress distribution at different speeds of measurements

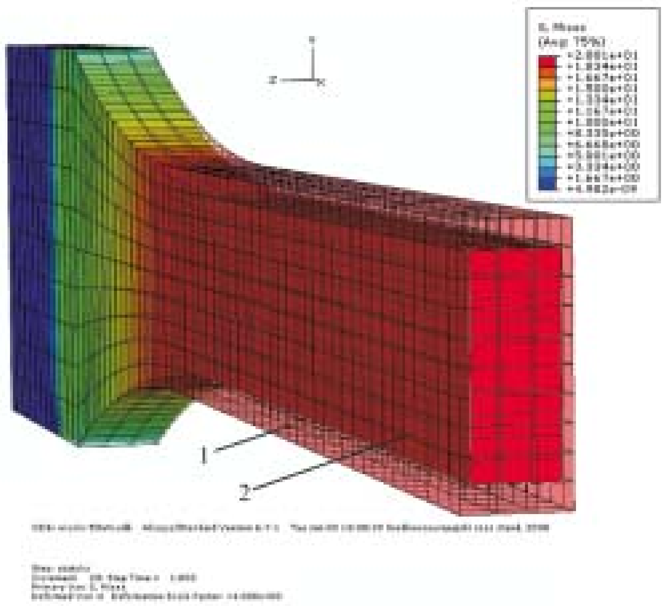

Fig. 5. Example of deformation of tested sample in the middle of its length: 1— before tensile test, 2 — after 5 % of deformation

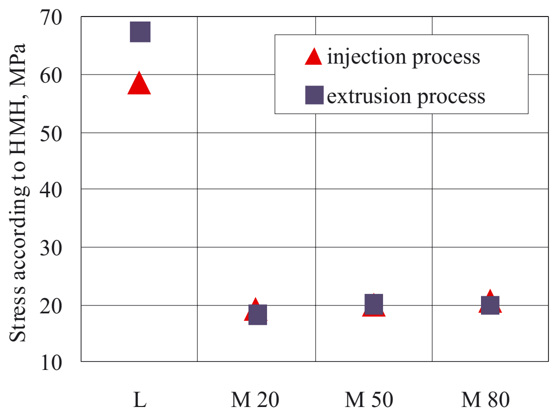

Fig. 6. Plot of dependence of reduced stress distribution on specimens according HMH hypothesis for the assumed characteristics of material: L — linear characteristics, M20, M50, M80 — the elastic-plastic characteristics at tensile rates 20, 50 or 80 mm/min, respectively

making possible to obtain the regular subdivision of model into the set of finite elements. The border conditions of model were defined by fixing the specimens on one end and by loading its free end, forced by dislocation assurring obtaining the 5 % level of the longitudinal strain (Fig. 4). The calculations with the finite element method, having assuming the different polymer material characteristics, show the essential differences both in respect to applied processing method, as well as to different tensile rates during the measure. The obtained results of calculations of models, in which the linear material characteristic was assumed, differ considerably from the models in which characteristic of elastic-plastic material was applied, obtained during the tests at equal speeds of measurement. Clear differences can be observed in the value of stress (Fig. 5 and Fig. 6), according to HMH hypothesis in the middle of sample length, and therefore in the area of its greatest strain.

CONCLUSIONS

Investigations of the strain function variations obtained at different tensile rates, for extruded or injected polyethylene samples showed the differences in absolute values with clear increase in stress with increasing strain rate. The carried out processes of extrusion or injection molding as well as the high strain rate at the tensile test did not confirm important differences in the degree of crystallinity of material tested. It was noticed that the method of polymer processing has a minor impact on the precision of simulation. Suitable material characteristics assumption for FEM analysis was of decisively greater importance. Therefore, the material characteristics introduced as input data for simulations should be defined in conditions most possibly close to the real loads and corresponding stresses occurring during the product operation. Realization of tests for high-density polyethylene products exclusively in the conditions described by suitable standards may lead to wrong conclusions. The values of obtained results show it clearly (Fig. 5). Moreover, on the basis of the results obtained it was confirmed, that in the case of parts produced from the tested material, an assumption of linear characteristics of material is a very large simplification, leading to essential divergences in the results of the numerical calculations. Even higher than 300 % of the values closed to the real ones. However, in analyzed case, the use of model of elastic-plastic material gives satisfactory results, showing large convergence with the results of experimental tests.

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