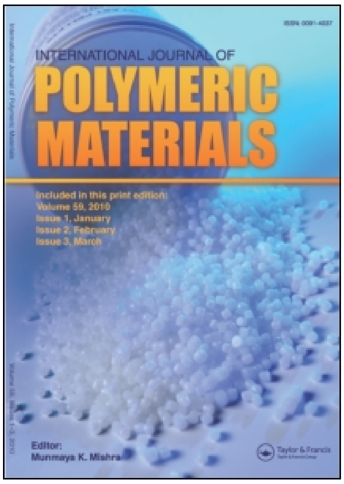

International Journal of Polymeric Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713647664

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To cite this Article He, Zongyan(1995) 'The Multiplication of Deformed Region and the Yield Model of Polymers', International Journal of Polymeric Materials, 28: 1, 199 — 209
To link to this Article: DOI: 10.1080/00914039508012103
URL: http://dx.doi.org/10.1080/00914039508012103

Intern. J. Polymeric Mater., 1995, Vol. 28, pp. 199–209
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The Multiplication of Deformed Region and the Yield Model of Polymers

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(Received September 6, 1994)

According to the analysis of the micro-deformation process of polymers, the author proposes a new concept of deformed region multiplication, from which an explicit elastic-plastic constitutive equation can be deduced. The characteristics of stress-strain curve in different conditions are discussed, which conform better the experimental results.

KEY WORDS Polymers, yield, constitutive relation, multiplication.

1. INTRODUCTION

Most ductile polymers can yield under different loading conditions.[1-2] A typical yield behavior is shown as Figure 1a: First, an upper yield stress point appears, it is followed by a plastic unstable stage which is governed by $d\sigma/d\varepsilon < 0$, and a constant stress platform stage governed by $d\sigma/d\varepsilon \approx 0$. Last, the strain hardening occurs when $d\sigma/d\varepsilon > 0$. Based on the author's experiments, another yield mode shown as Figure 1b can be obtained. It has the upper and lower yield stresses but without the yield platform. Considering different materials and initial conditions, we can get additional yield modes. In Figure 1c, there is a point of inflexion without a decrease in stress. In Figure 1d, the yield platform exists but without the upper yield stress. In some cases, the actual stress-strain curve has neither an extreme nor an inflexion point (Figure 1e). Adopting the method used in metals, the stress which results in $0.01 \sim 0.03$ residual strain is regarded as the yield stress.

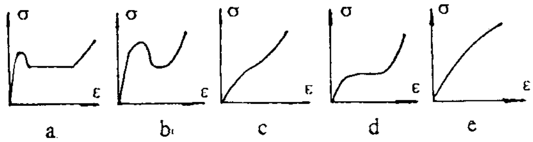

FIGURE 1 Several typical yield modes.

Researchers have proposed many theories to explain the yield phenomena. Consider suggested that the yield is a geometrical unstable effect based on the necking-down of the specimen. This theory can not explain the yield without necking-down under pressure.[2-4] Many people think the intristic mechanism of yield is the local increase of temperature in the deformation process. The platform of yield shows an equilibrium between the created heat and the transmitted heat in the region of the specimen.[5-7] But the temperature may not be the most essential reason, because a very slow loading under constant temperature can also cause an obvious upper yield point.[8]

One of the micro-yield theories suggests that the external load causes molecules to flow in one direction, the yield stress is the stress at which the strain rate is equal to the plastic strain rate $\dot{\varepsilon}_p$ governed by the Erying's equation. On the basis of this theory, many models and methods were developed and the following formula can be deduced[1]:

$$\frac{\sigma_s}{T} = \frac{R}{V}\left[\frac{\Delta H}{RT} + \ln\frac{\dot{\varepsilon}_s}{\dot{\varepsilon}_0}\right] \tag{1}$$

where, σ_s is the yield stress, $\dot{\varepsilon}_s$ is the corresponding strain rate, ΔH and V are the activation energy and activated volume, T is the absolute temperature and R is a physical constant. The formula shows that there is a linear relationship between σ_s/T and $\ln\dot{\varepsilon}_s$.

Based on the concrete mechanism of flow, a model of polymer chain rotation conformation was proposed.[9,10] It suggests that the yield flow of molecule is caused by the rotational change of polymer chain from the lower energy state of anti-form to the higher energy cis-form state. When the proportion of the cis-molecule is sufficiently high, the macro-yield occurs.

Argon advanced another model of molecular flow.[10,12] He suggested that the resistance of retarding the formation of double twisted chain is the elastic interaction between the chains. The yield process needs not only the formation of the double twisted chain but also the coordination of the neighbour chains. From this model, the relation between the yield shear stress τ_s and strain rate $\dot{\gamma}_s$ can be obtained:

$$\tau_s = \frac{0.102G}{1-\nu} + \frac{16 \times 0.102KT}{3\pi\omega^2 a^3}\ln\frac{\dot{\gamma}_s}{\dot{\gamma}_0} \tag{2}$$

where, G is the shear modulus, ν is the poisson's ratio, a is the radius of the molecule chain, ω is rotation angle of the segment of the Chain and K is a physical constant.

Bowden analysed the yield sliding process of the non-crystalline polymers from the analogy of expanding dislocation loops.[13] The yield will occur when the radius of the loop reaches a critical value and the formation energy of the loop decreases with increasing stress.

The free volume theory suggested that material may expand under stress field, which enhances the possibility of segmental movement of the chain which results in yield. Some other theories indicated that many yield processes are caused by the micro-voids and micro-crack when the material expands.[14-16] Many experiments show that in the yield process, the molecular chain fracture, void formation, molecular orientation and molecule chain sliding occur simultaneously. The more brittle a material is, the larger is the effect of the cracks and voids, and the tougher a material is, the larger is the contribution of molecular orientation and sliding.

The present author suggests that the yield mechanism of polymers does not depend only on the micro-structure reorganization revolution, but also on the process dynamics of the deformation region in the entire specimen. Thus, a yield model based the multiplication of deformed region will be proposed and the corresponding elastic-plastic constitutive equation will be deduced.

2. PHYSICAL MECHANISM OF DEFORMED REGION'S MULTIPLICATION

Deformed region multiplication means that the deformation in a small region of the specimen can cause the deformation of its neighbour regions, which will make the farther regions deformed. In this concept, the deformation can expand to the whole specimen.

At the beginning of loading, the polymer is in the elastic state. Then, due to the unavoidable geometric and structural non-uniformities, the plastic deformation occurs only in some stress concentration regions. The geometric non-uniformity is created during the preparation of the specimen, while the defects distributed at random will cause the structural non-uniformity. With the increase of stress, the plastic deformation in these regions causes new stress concentrations, which will make of the plastic deformation autocatalytically. On the molecular scale, the material is also inhomogeneous. The weak regions may contain a large amount of chain ends, untwisted section between the chains, and the sections-chains which are vertical to the stress direction. Especially, when the chain is fractured, this position will become a new weak region.[17] Under loading, these regions will be damaged first and formed micro cracks or voids, which will weaken their adjacent regions. This mechanism of weak region multiplication is common in brittle materials.

The thermal effect in the deformation process will now be considered. When the strain rate is over $5 \times 10^{-3}\ S^{-1}$, the temperature increase can not be neglected.[7] The heat may come from the work of the external forces, the decrease of entropy due to the molecule chain orientation and the internal energy release. The infrored photography shows that the temperature in the shoulder region of the specimen is the highest (Figure 2). It means that there is a great quantity of heat in front of the plastic deformed region, and the adjacent elastic regions can be softened and create more heat resulting from plastic deformation, so the additional elastic regions will be softened until the plastic deformation expands to the whole specimen.

Another possible effect is that the radicals caused by the fracture of stressed molecules can become the catalyst for the fracture of the adjacent molecules.[18] This kind of failure can also be regarded as one of the micro-mechanisms of deformed region multiplication.

On the basis of above analysis, the author proposes that the plastic deformation of polymers begins in some stress concentration positions and expands gradually

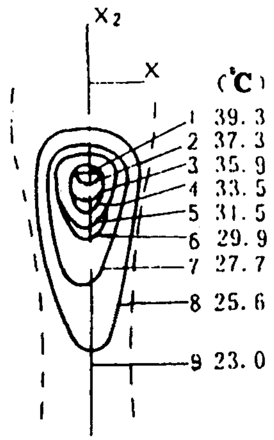

FIGURE 2 The distribution of temperature in a specimen.

by a mode of plastically deformed region multiplication. The dynamic characteristics of this process may result in the yield and cold tension. Hearle has indicated[19] that the yield may concentrate on the shoulder regions or other local regions. The decrease of the yield stress may be caused by the changes of the micro-structure. That is to say, once the structure starts to fail, the deformation of adjacent structure elements may be easier, because the plastic deformation causes the material to heat.

3. FORMULATION OF THE CONSTITUTIVE EQUATION

The following assumptions were applied to the deformed region's multiplication

1) The multiplication rate is defined as the increment per unit volume of deformed region in unit time. It is a parameter related with the type of material.

2) The multiplication space (specimen's volume) is limited, the material is isotropic and the dimensions of the specimen in three directions are of the same order.

3) The time for keeping the deformed region's multiplication is so long that the adjacent region can fully deform.

4) The time lag of the multiplication process is negligible. This is based on the hypothesis that the velocity of heat flow is fast.

5) The induction period of multiplication (from initial loading to the beginning of plastic deformation in some regions) is almost zero.

6) The multiplications in different deformed regions are independent of each other.

7) The multiplication damping and driving force are all constants during the whole deformation process.

8) The plastic deformation starts only at one position with highest stress concentration.

On the basis of the above assumptions, the multiplication rate $d\omega/dt$ of the volume of the plastic deformed region is a function of the volume ω. By Taylor's series, it can be expressed as:

$$\frac{d\omega}{dt} = F(\omega) = C_0 + C_1\omega + C_2\omega^2 + \ldots \quad (3)$$

when $\omega = 0$, $d\omega/dt = 0$, therefore $C_0 = 0$. With t increasing, $d\omega/dt$ increases from zero and reaches its maximum at a certain time, then decreases to zero due to the limitation of the multiplication space. So, there are two real roots for $F(\omega)$. By selecting three terms in the right side of (3) we obtain:

$$\frac{d\omega}{dt} = C_0 + C_1\omega + C_2\omega^2 = b\omega\left(1 - \frac{\omega}{W}\right) \quad (4)$$

The integration leads to

$$\omega = \frac{W}{1 + e^{a-bt}} \quad (5)$$

when $W = \omega$, $d\omega/dt = 0$ and W is the whole volume of the specimen. $\omega_0 = \omega|_{t=0} = W/(1 + e^a)$ is the volume of deformed region at initial time, and

$$a = \ln\left(\frac{1}{C} - 1\right) \quad (6)$$

is a parameter related with ω_0. Here, $C = \omega_0/W$ is the initial volume ratio.

From (4), we get:

$$\frac{1}{\omega} \cdot \frac{d\omega}{dt} = b\left(1 - \frac{\omega}{W}\right) = B \quad (7)$$

Here, B is the actual multiplication rate for the above conditions. It will decrease when ω increases, which shows the limitation of the multiplication space. If the space is infinite, $B|_{\omega\to\infty} = b$. Therefore, b is a multiplication rate regardless of the space limitation. We assume it is a material constant.

In a real case, the effect of external stress σ must also be considered. Under uniaxial loading, the larger the stress, the easier the multiplication. From this it follows that σ is proportional to ω, or proportional to the multiplication rate. The calculation shows that the second assumption is more reasonable. Therefore,

$$\frac{d\omega}{dt} = b(\alpha\sigma + \beta)\omega\left(1 - \frac{\omega}{W}\right) \tag{8}$$

And

$$\omega = \frac{W}{1 + e^{a - b(\alpha\sigma + \beta)t}} \tag{9}$$

Here α and β are constants determined by experiments.

The displacement H of the crosshead of the tension machine is the sum of the elastic deformation P of the tension machine and the plastic deformation Q of the specimen:

$$H = Vt = P + Q = \frac{\sigma_s}{K} + Q \tag{10}$$

Here, V is the velocity of the crosshead, t is the time of deformation, K is the elastic constant of the tension machine and S is the cross area of the specimen.

For simplification, we assume that the contribution ψ of unit volume of the deformed region to the macro-extension of the specimen is a material constraint. Therefore,

$$Q = \frac{\sigma l}{E} + \omega\psi \tag{11}$$

where E is the elastic modulus, l is the length of the elastic region along the tension direction, l can be expressed as

$$l = \frac{W - \omega}{S} \tag{12}$$

From (9)–(12) it follows

$$Vt = \frac{\sigma S}{K} + \frac{W\{\psi + \frac{\sigma}{ES}\exp[a - b(\alpha\sigma + \beta)t]\}}{1 + \exp[a - b(\alpha\sigma + \beta)t]} \tag{13}$$

It is easy to rewrite the above relation between σ and t into stress-strain relationship. In fact, under constant velocity of loading, the two types of relation curves have similar shape.

If the elastic deformations of the tension machine and the specimen are neglected, we can get from (13) the following formula:

$$\sigma = \frac{a - \beta bt - \ln(W\psi - Vt)}{\alpha bt} + \frac{\ln(Vt)}{\alpha bt} \tag{14}$$

4. DISCUSSION ON THE σ-t CURVE

From (14), we can obtain:

$$\frac{d\sigma}{dt} = \frac{1}{\alpha bt^2}\left[\ln\left(\frac{W\psi}{Vt} - 1\right) + \ln\frac{W\psi}{W\psi - Vt} - a\right] \tag{15}$$

By selecting $d\sigma/dt = 0$, we obtain

$$e^{-x} = a - 1 - x \tag{16}$$

where $x = \ln(W\psi/(Vt) - 1)$. If $y_1 = e^{-x}$, $y_2 = a - 1 - x$, the relation between y_1 and y_2 has three possibilities in Descartes coordinates:

1) When $a < 2$, the two curves of y_1 and y_2 do not intersect (Figure 3a), so there is not solution for eqn. (16). From (6), $C = \omega_0/W > 1/(1 + e^a) = 11.9\%$, i.e. when initial volume ratio is bigger than 12%, there are no extremes (or upper and lower yield stresses) in the $\sigma - t$ curve described by eqn. (14).

From (15) and $d^2\sigma/dt^2 = 0$, an equation of variable t can be obtained:

$$\frac{W\psi(2Vt - W\psi)}{(W\psi - Vt)^2} = 2\left[\ln\left(\frac{W\psi}{Vt} - 1\right) + \frac{W\psi}{W\psi - Vt} - a\right] \tag{17}$$

According to these calculations, there is also no solution for (17) when $a < 2$. That means, the curve has no inflection point. So the constitutive relation from (14) describes the yield mode in Figure 1e.

2) When $a = 2$, there is an intersection point between y_1 and y_2 (Figure 3b). The real root of eqn. (16) is $x = 0$, when $t = W\psi/(2V)$. From (17), this point corresponds to the inflection point of the $\sigma - t$ curve, but not an extreme. Con-

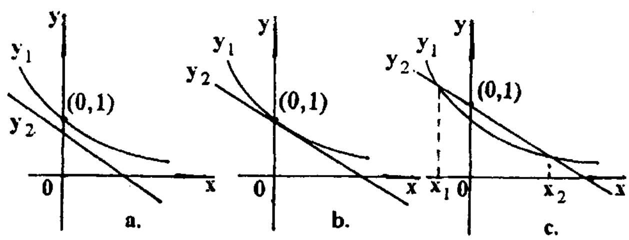

FIGURE 3 Three possible relations between the curves of y_1 and y_2.

sequently, when the initial volume ratio approaches 12%, the constitutive eqn. (14) gives the yield mode shown in Figure 1c.

3) If $a > 2$, there are two intersection points between y_1 and y_2 (Figure 3c). When $x < x_1$, $y_1 > y_2$, i.e. $e^x > a - 1 - x$; $d\sigma/dt > 0$. This shows that before the tension time t_L, corresponding to the first intersection point, $\sigma - t$ curve is upward. When $x_1 < x < x_2$, $y_1 < y_2$; $d\sigma/dt < 0$, this shows the stress will decrease. When $x_2 < x$, the tension time is larger than t_u corresponding to the second intersection point and $d\sigma/dt > 0$. The curve will go up again. So, t_L and t_u are the time for upper and lower yield stresses, respectively. The constitutive eqn. (14) describes the yield mode shown in Figure 1b.

According to the preceding analysis, we can see that a well machined specimen with uniform micro-structure has a small region of plastic deformation at initial time, therefore, a is small and an obvious yield and plastic unstability will exist. If the fabrication is crude, or the micro-structure is non-homogeneous, there may be no upper and lower yield stresses. This was verified by experiments.

On the other hand, the configuration and size of the specimen can also affect the stress-strain curve. If the size in one direction is much smaller than in the other two directions, the specimen can be considered as a two dimensional plate. When the plate length and width are of the same order, it may form a deformed region in two dimensions. We assume,

$$\frac{d\omega}{dt} = b\theta\omega^{1/2}\left(1 - \frac{\omega}{W}\right) \tag{18}$$

Here, θ is the shape factor of the region. If the region extends circularly, $\theta = 2\sqrt{\pi}$. If it is a rectangle with the ratio k between its length and width, $\theta = 2(k^{1/2} + k^{-1/2})$. We assumed θ as a constant during the deformation process. From (18), we get

$$\omega = W\left(\frac{c'e^{C''t} - 1}{c'e^{C''t} + 1}\right)^2 \tag{19}$$

where $C' = (1 + C^{1/2})/(1 - C^{1/2})$, $C = \omega_0/W$, $C'' = b\theta$. Assuming $b = b_0(\alpha\sigma + \beta)$ and neglecting the elastic deformation, we obtain

$$\sigma = -\frac{\beta\lambda t + \ln c'}{\alpha\lambda t} + \ln D \tag{20}$$

where $\lambda = b_0\theta$, $D = (1 + n^{1/2})/(1 - n^{1/2})$, $n = Vt/\psi W$.

If the size in tensile direction is much larger than those in other two directions, the initial three dimensional extension of deformed region will soon transform into one dimensional multiplication along the tensile direction. The deformation band will sweep the entire specimen shown in Figure 4. Let the length of the specimen be L, cross area be S, the length of deformed region be l. Because only the front of the deformed region can make its neighbor region deform, the multiplication

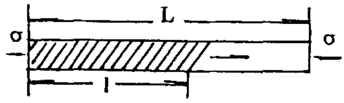

FIGURE 4 The extension of deformation band.

velocity $d\omega/dt = Sdl/dt$ will not be proportional to the whole volume of the deformed region. It should be assumed that the larger the external stress, the faster the increasing of the length l is. Consequently,

$$\frac{d\omega}{dt} = S\frac{dl}{dt} = b_0(\alpha\sigma + \beta) \tag{21}$$

Regarding $dl/dt > 0$ and $l = 0$ as the initial conditions after the transformation from three dimensional multiplication to one dimensional extension, it follows that

$$\sigma = \frac{VS - \beta\psi b_0}{\alpha\psi b_0} \tag{22}$$

This shows that when a one dimensional multiplication occurs, the stress will be constant. The corresponding stress-strain curve has an upper yield point and a yield platform, then, the stress will go up again after the deformation band extends to the whole specimen. So, most of specimens under uniaxial loading can have the yield mode shown in Figure 1a.

If the fabrication is crude or the micro-structure is non-uniform, the curve only has a platform without upper yield stress point. This mode is shown in Figure 1d.

It must be pointed out that the yield platform can be regarded as the equilibrium between the strain softening and the orientational intensification because ψ has a limited value.

For comparing with the experiments, we consider the strain rate:

$$\dot{\varepsilon} = \frac{d\varepsilon}{dt} = \frac{1}{L}\cdot\frac{dL}{dt} = \frac{V}{L} \tag{23}$$

So

$$V = L\dot{\varepsilon} \tag{24}$$

From eqn. (14), we obtain

$$\sigma_s = \frac{a - \beta bt_s}{\alpha bt_s} - \frac{\ln(W\psi - Lt_s\dot{\varepsilon})}{\alpha bt_s} + \frac{\ln(Lt_s\dot{\varepsilon})}{\alpha bt_s} \tag{25}$$

where σ_s is the yield stress, t_s is the occurring time of σ_s. If $\dot{\varepsilon}$ is not too large and t_s is sufficiently small, there is a linear relation between σ_s and ln $\dot{\varepsilon}$, which is

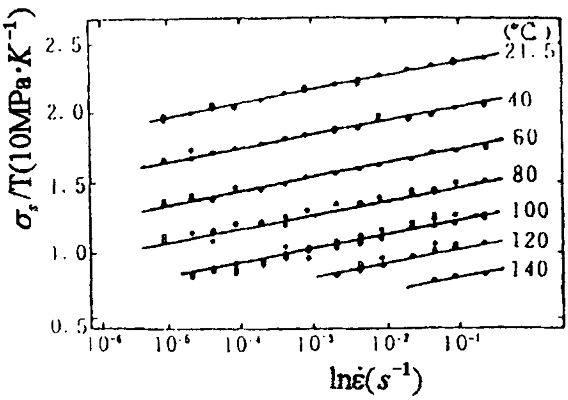

FIGURE 5 The relationship of σ_s/T − $\ln\dot{\varepsilon}$.

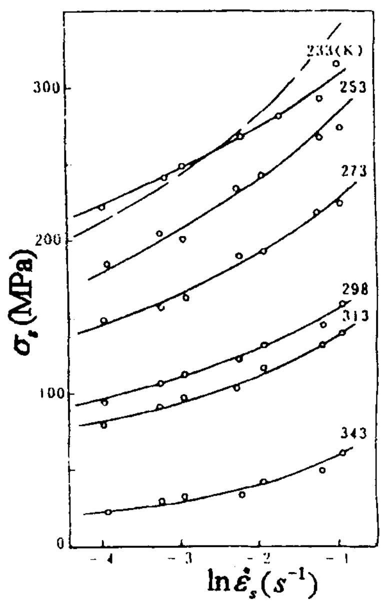

FIGURE 6 The relationship of σ_s − $\ln\dot{\varepsilon}_s$.

consistent with the microscopic yield models represented by formulas (1) and (2), and is consistent with the experimental results[20] shown in Figure 5.

If $\dot{\varepsilon}$ is large, we will find that the relation of σ_s − $\ln\dot{\varepsilon}$ is not completely linear. With the increasing of $\dot{\varepsilon}$, σ_s is larger than that of the value calculated from linear relation. Figure 6 is the experimental results of Reference 21, which can be represented by eqn. (25).

In the above constitutive equations the effect of temperature is not considered. It is expected that it will affect the multiplication rate.

5. CONCLUSIONS

1) The plastic deformation in polymer starts at a small volume element. By the mode of multiplication, the deformed region will extend to the whole specimen. The front of the region forms the deformation band.

2) The phenomena of yield and cold flow in polymers are related with the multiplication process of the deformed region.

3) Under some conditions, a simple constitutive relationship can be deduced based on the multiplication process. Some quantitative descriptions on several typical yield modes can be derived from different initial state, size and shape of the specimen.

4) The relation between yield stress and strain rate based on this model is consistent with the microscopic yield theories and the experimental results reported in literature.

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