FINITE ELEMENT MODELING OF CREEP IN POLYMER/CNT NANOCOMPOSITES

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ABSTRACT

How to model creep and the method for obtaining the most precise creep strain curves versus time for reinforced polymers by carbon nanotube have provided backgrounds for this study. Many works have been done to physical modeling for this kind of nanocomposites and different methods such as molecular dynamic have been applied but each of them confronted to some restrictions which these problems have been solve by finite element method that presents in this paper. Experimental modeling in large scale have been done by power law models but they didn’t lead to predictive results, thus, in this paper it was tried to model the viscoelastic creep in mentioned nanocomposites using parameters of the constituent materials and it was also tried to present finite element method to obtain the desired purpose.

Keywords: Creep, finite element method (FEM), carbon nanotubes (CNT), polymer/CNT nanocomposites.

Polymeric nanocomposites have attracted many attentions in science and engineering because of their unique characteristics during last decades. On the other hand creep as a time related phenomenon is an important issue for application in which need long time durability and reliability (Aifantis, 1987). Creep can also define as an increased growing strain within a material exposed to a constant load and stress (Arvidsson, 2004). This phenomenon can be surveyed for a sample of special material by creep test machine, but we want to extend the analysis domain for example for a composite part, we need a model that predicts the creep of nanocomposite using properties of constituent materials.

Molecular dynamics simulations have been done for modeling and simulation of some properties of nanocomposites and led to significant results. For example, a simulation did for prediction of elastic properties for CNT/polyimide composites with different volume percent and their stress-strain behavior have been studied during this modeling process (Odegard, 2002; Francland, 2003) but, it was cleared that molecular dynamic simulation are limited to small time scales which are a challenge for long time assessments, so some investigator attempt to large scale modeling (Liu, 2005). At this condition, boundary element method and finite element method have introduced and difference between determined (Liu, 2003), but still, there are space for applicable research for these two methods to analysis of a given composite, thus finite element method selected to assessment of creep behavior and analysis of creep strain that create in CNT reinforced polymeric nanocomposites.

Creep is primary behavior of viscoelastic materials which is a time depended deformation in constant stress. Therefore, focusing on the elementary models that created for this process is logical. Power-

MODELING

Introduction to creep and power-law creep relations

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law model is one of the suitable models for creep; fundamental equation for creep models has following quality form (Horvath, 1998):

\[ \varepsilon_c = \varepsilon_0 + \varepsilon(t) \]

Where:
- \( \varepsilon_c \): total creep strain
- \( \varepsilon_0 \): immediately strain from applied stress (elastic part of strain)
- \( \varepsilon(t) \): time related component of creep in time after applied stress

It is assumed that stress is applied instantly, its size is constant and its duration is permanent. An exception for Equation (1) includes elimination \( \varepsilon_0 \) (immediately strain) for simplicity of related components, stress surface and time which its amount is very smaller than creep component \( \varepsilon_c \).

Equation (1) can be rewritten in a more generally form and it is known general power-law model:

\[ \varepsilon_c = \varepsilon_0 + A\sigma^n t^m \]

Where, \( \sigma \) is uniaxial deviation stress and \( m, n \) are dimensionless power parameter. More details about dimensionless parameters are shown in table 1.

**Table 1. Creep power parameters**

<table>
<thead>
<tr>
<th>A</th>
<th>&gt; 10^{-27}</th>
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<tr>
<td>n</td>
<td>&gt; 0</td>
</tr>
<tr>
<td>m</td>
<td>-1 &lt; m &lt; 0</td>
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</tbody>
</table>

A and n should be positive. For creep strain rates, value of A may be very small, However if its value be less than \( 10^{-27} \), numerical problems may be cause error in calculations (Arvidsson, 2004).

**Modeling**

Regarding to desired purpose, method should be selected that lead to most precise results so, finite element modeling with ABAQUS software was used for this survey. It is tried to modeling the representative volume element (RVE) of polymer and with determined boundary condition, uniform tension stress will be applied and finally finding creep strain after meshing of model. Again, this representative volume element is used with exception that CNT, with maintain interface (boundary between matrix and reinforcement) between elements. A tensile stress is applied and its creep strain-time diagram is obtained. Polycarbonate has been considered as matrix in a representative volume element polymer in which properties of materials as inputs for software are shown in table 2 and 3 (Odegard, 2002).

**Table 2. Elastic properties of polycarbonate**

<p>| | |</p>
<table>
<thead>
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<tr>
<td>E</td>
<td>2.4 Gpa</td>
</tr>
<tr>
<td>v</td>
<td>0.3</td>
</tr>
</tbody>
</table>

**Table 3. Properties of carbon nanotube**

| E | 450 Gpa |

Creep properties for this model are shown following (Arvidsson, 2004; Ouyang)

**Table 4. Creep properties for polycarbonate**

| A (Power law multiplier) | 3.11 E -15 |
The boundary condition in one side of representative volume element and the applied tensile stress in the other side are considered as shown in figure 1.

\[
    f_{CNT} = \frac{\pi \left( h_{CNT} + \frac{h_{vdw}}{2} \right)}{A_{cell}}
\]

Where, \( h_{vdw} \) is balance van der waals distance between CNT and matrix, and \( A_{cell} \) is cross section area of unit cell. Separation distance of van der waals depend on interface nature of polymer/CNT.

**RESULTS AND DISCUSSION**

After steps for modeling, results for creep strain vs time diagram is obtained. As can be seen in figure 3, adding single wall CNT decreases creep strain of polymer. It should be said that SWCNT only take 1% volume fraction of nanocomposite.

Figure 4 shows comparison between results from modeling of volume element for polymer with FEM and other methods which diagrams are presented comparatively for demonstration of validation and advantage of this method.
Figure 5 shows comparisons of creep diagrams for different volume fractions of CNT. As can be seen in this figure, creep strain decreases with increasing volume fraction of CNT.

Figure 5. Creep diagram of volume element of polymer/ CNT with different volume fractions using FEM.

In figure 3 and 5, we can see decrease of creep strain for polymer with addition CNT compared with pure polycarbonate. Figures 6 to 10 show comparison between results from FEM modeling and Findley diagram from experimental results.

Figure 6. Comparative diagram for creep of volume element of polymer/ CNT 0%

Figure 7. Comparative diagram for creep of volume element of polymer/ CNT 1%

Figure 8. Comparative diagram for creep of volume element of polymer/ CNT 3%

Figure 9. Comparative diagram for creep volume element of polymer/ 5%

Figure 10. Comparative diagram for creep volume element of polymer/ CNT 7%

CONCLUSION

Advantage of finite element method relative to the other methods such as molecular dynamics is that it can be used for long time intervals which are common in creep analysis. For example, for estimation of service duration of nanocomposites that need long term duration in industry, time limitations in analysis is an important restriction for precise survey in molecular dynamics analysis. See diagrams and compare their results from other method, suggests this method is more precise and reasonable. As it was expected, finite element analysis shows that creep strain decreases when CNT is added and resistance to creep increases.
REFERENCES


Ouyang F, 2005, Abaqus implementation of creep failure in polymer matrix composites with transverse isotropy, Mas. of Sci. thesis


