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**Micromechanics of particle-modified semi-crystalline materials**

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**Introduction**

The toughness of semi-crystalline materials can be significantly improved by the addition of second phase particles. A multi-scale numerical model is developed to investigate the role of the microstructure on the macroscopic behavior.

**Methods**

A distinction between three different scales is made. The constitutive properties of the material are characterized at the microscopic scale. At this scale, the individual crystallographic lamellae and amorphous layers are identified.

<table>
<thead>
<tr>
<th>Microscopic level (constitutive level)</th>
<th>Mesoscopic level (aggregate level)</th>
<th>Macroscopic level (toughening level)</th>
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<td>Composite inclusion model</td>
<td>Finite Element Modeling</td>
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<td>crystalline phase</td>
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<tr>
<td>amorphous phase</td>
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</tbody>
</table>

**Figure 1** Different length-scales in particle-modified material.

At the mesoscopic scale, an aggregate of individual phases is formed. To bridge to this scale, a layered two-phase composite inclusion (CI) model [1] is formulated. The inclusion-averaged fields are related to the fields of the aggregate by a hybrid interaction law.

**Results**

**Unfilled HDPE**

In unfilled material, a preferred orientation with parallel lamellae, with the normals in the loading direction, is found to prevent the occurrence of localization.

**Figure 3** Preferred orientation with different loading angles.

**Filled material**

**Anisotropic Hill model**

The use of a Hill-type plasticity model shows that a surface-induced anisotropy ($R_{12} = R_{13} = 1/5$) can potentially effectively suppress localization in particle-modified systems, as can only be represented by an irregular RVE [2], and has a distinct influence on the triaxial stress state, which is described by an axisymmetric RVE with a regular (BCT) stacking [3].

**Figure 4** Irregular plane strain ($\bar{\varepsilon}_p^{\text{eq}}$) and axisymmetric ($\bar{p} / \tau_0$) RVEs with isotropic and anisotropic (Hill) material.

**Composite inclusion model: HDPE**

A surface-induced orientation causes a somewhat more dispersed occurrence of plastic deformation. Moreover, the local anisotropy leads to a reduction of the triaxial stress state.

**Figure 5** Irregular plane strain ($\bar{\varepsilon}_p^{\text{eq}}$) and axisymmetric ($\bar{p} / \tau_0$) RVEs with the CI model with random and surface-induced orientations.

**Conclusions**

- Changing the microstructure can prevent the occurrence of localization in unfilled HDPE.
- The irregular and 3D nature of particle-modified systems requires the use of both irregular plane strain and regular axisymmetric RVEs.
- A surface-induced anisotropy has a small influence on the plastic deformation and the triaxial stress state.

**References:**