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Effective Properties of Nano-Filled Polymers

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ABSTRACT

If polymers come in contact to other materials boundary layers are formed. In theses boundary layers, often called interphases, the mechanical properties of the polymer differ from its bulk properties. The formation of the boundary layers leads to size effects in polymer bonds [1,2]. This effect is even more important in nano-filled polymers because the small fillers form a very large internal surface.

In the model developed in [1] the formation of the boundary layer is described by an extended continuum mechanical model. Therefore an additonal degree of freedom is introduced. This structural parameter drives a phase transition from the bulk material to the interphase material with different properties. In [2] it is shown that the extended model can be fitted to experimental data very well.

In the present contribution the nano-filled polymer is investigated on the scale of the representative elementary volume (REV). On the microscale the individual filler particles are assumed to be elastic while the polymer is described by the extended theory mentioned above. Therefore, a boundary layer forms around each particle. After a numerical homogenisation over the REV the effective properties of the filled polymer are obtained as functions of the filler volume fraction and of the filler size. Therefore, a strong size effect with respect to the size of the filler is observed, i. e. the effective properties change if the filler particles become smaller even if the volume fraction is kept constant. The main advantage of the applied model can be seen for very small particles. In this case the internal surface becomes very large and the boundary layers around the individual filler start to interact. This interaction is included in the micromechanical model in a natural way.

REFERENCES

[1] S. Diebels, M. Johlitz, H. Steeb, A. Chatzouridou, J. Batal and W. Possart. “A continuum-based model capturing size effects in polymer bonds.” *Journal of Physics: Conference Series*, Vol. **62**, 34–42, 2007.

[2] M. Johlitz, H. Steeb, S. Diebels, J. Batal and W. Possart. “Experimental and numerical investigation of size effects in polyurethane adhesive sealings”. *Technische Mechanik*, accepted for publication, 2007.