MODELING AND PREDICTION OF MECHANICAL AND OPTICAL PROPERTIES BASED ON KEY PARAMETERS OF CRYSTALLINE STRUCTURE

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The properties of the semicrystalline materials are depending on their complex crystalline structure. Isotactic polypropylene (iPP) is a semicrystalline commodity polymer, which develops dynamically nowadays, because its properties can be modified in wide range throughout the modification of its crystalline structure. The stiffness and optical transparency of iPP are the most important properties from the point of view of several applications. Although the key parameters of the crystalline structure, which determines the aforementioned properties are known in the literature, but the quantitative modeling is difficult and time consuming procedure if possible at all. In fact the number of models, which link the crystalline structure to the properties, is limited in the open literature. Accordingly, prediction of upper limit of stiffness and the best achievable optical transparency is an open question in general.

In the present work we focused on the prediction of upper modulus limit of iPP and the quantitative description of haze based on parameters of crystalline structure. A former model equation was used to describe stiffness [1] and the new model was developed to describe the light scattering in the semicrystalline polymers. The accuracy of the models was tested on several set of samples and good agreement was found between the calculated and measured modulus values, however the accuracy of the haze prediction need to be improved in the future studies. The results indicate clearly that these properties could be improved only if the molecular structure of the polymer is designed to the unique properties.

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[1] Menyhárd, A., Suba, P., László, Z., Fekete, H. M., Mester, Á. O., Horváth, Z., Vörös, G., Varga, J., Móczó, J., Direct correlation between modulus and the crystalline structure in isotactic polypropylene Express Polym. Lett. 9. 308-320 (2015)