INFLUENCE OF BRANCH DEFECT ON ELASTIC PROPERTIES OF DENDRIMERS

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At this work influence of branch defect on elastic properties of poly(propylene imine) dendrimers of the 7th generation are studied. Previously compression diagrams were obtained and stiffness coefficients were determined for ideal dendrimer macromolecules, placed between planar plates, using molecular dynamics method [1]. However, in practice dendrimers don't possess perfect structure in all cases. A certain percent of molecules contain defects of chemical synthesis.

Poly(propylene imine) dendrimers consist of four-functional core (**>N–$(CH_2)_4$–N<** group), branching centers (tree-functional nitrogen atoms **–N<**), spacers (composed of tree methylene groups,**–$(CH_2)_3$–)**, and terminal groups (imines **–NH_3**). Starting with first generation the molecules were assembled layerwise, at that a number of branching defects (stubs) arranging in random manner was given at each intrinsic layer. A stub is a chemical group replacing a regular spacer and, in that way, stopping a further growth of a corresponding branch. In our case the stub is a hydrogen atom. Seven molecules were analyzed: a dendrimer without defect (G7); six dendrimers with one defect at one generation (G7di – defect at i^{th} generation). Macromolecules of the perfect dendrimer and ones with branch defects were constructed using the generator of molecular structures [2].

In the starting state, the adsorbed dendrimer molecule is in the state of equilibrium at the immobile surface while the second surface is removed to such a distance as to make its interaction with the macromolecule negligibly small. The mobile wall moves at a constant velocity compressing the dendrimer, and then, it moves back at the same velocity.

All analyzed dendrimers in adsorbed state looked as a half-sphere. Height of the dendrimer with the defect at first generation (G7d1) was about 33 A, whereas for the rest dendrimers it was greater - 37.5± 1.5 A. Reversible deformation was observed for all considered molecules. During compression dendrimers become flat, but when unloading they reshape their own form. Obtained dependences of a force F on distance h between plates are exponential with the same inclination of line.

References

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