Thermal properties of polymers via molecular dynamics simulations and thermal analysis

Kalle J. Tuomi[a], Tuuva Kastinen[b], Benjamin J. Lear[c], Tapio T. Rantala[d], Terttu I. Hukka[a,*]

[a] Chemistry and Advanced Materials, P.O. Box 541, 33014 Tampere University, Finland.

[b] Department of Chemistry and Materials Science, Aalto University, P.O. Box 16100, 00076 Aalto, Finland.

[c] Department of Chemistry, 104 Chemistry Building, Penn State University, University Park, PA 16802, USA.

[d] Department of Physics, 33014 Tampere University, Finland.

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Differential scanning calorimetry (DSC) is a thermo-analytical method that enables the quantitative determination of the thermally induced physical changes occurring in the sample during the heating or cooling process over the glass transition and melting regions. On the other hand, molecular dynamics (MD) simulations is a computational tool that allows the studies of the thermal properties of materials remotely also outside the laboratory.

In this work, the thermal properties of traditional and biopolymer materials have been investigated via MD simulations using the GROMACS2020 suite of programs. The implementation of a computational tool such as a MD simulation package, within a six months' Master of Science work, is a challenge by itself, but the implementation and correct usage of the MD simulations for tackling the thermal properties of materials is another. In this research, the responses of polymer materials, which are heated or cooled, are simulated by MD and the results compared to experimental findings. First, the behavior of the poly(oxyethylene) is studied over the glass transition region, similarly to the C. Wu's work, to verify the correct application of the simulation method. The verified method is then adapted to other polymeric systems. Comparative experimental studies will be carried out with DSC.

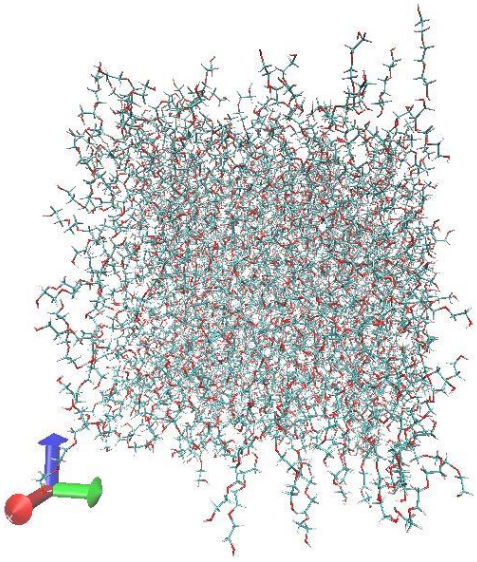

Figure 1. *Energy minimized poly(oxyethylene) trimers in a cube. Starting structure for the amorphous morphology.*

tuuva.kastinen@aalto.fi