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Physical understanding of the bulk modulus of polyisoprene by molecular dynamics simulations JULIE DIANI, LIM, ENSAM Paris, BRUNO FAYOLLE, PIERRE GILORMINI, MELAC TEAM — The temperature dependence of the Young's modulus of amorphous polymers has been explained well in the literature, however, the moderate drop of the bulk modulus of a factor 2 or 3 is still not fully understood and the question of a possible entropic contribution to the bulk deformation is still open. In this work, we propose to address the question of the physical source of the bulk modulus of the polyisoprene cis1-4, using molecular dynamics simulations. Using Material Studio MD simulations software, we built several periodic virtual polyisoprene. The materials were submitted to volume contractions at various temperatures. During the simulations, we monitored among other parameters, the volume, the pressure, the temperature, the bonded, nonbonded and kinetic energies of the cell. These data were used in a classical thermodynamics analysis to assess the physical source of the bulk modulus below and above the glass transition temperature. The results showed that the Van der Waals interactions control the bulk modulus below the glass transition. Above the glass transition the internal energy contribution to the bulk modulus is driven by the Van der Waals interaction but a non negligible entropic contribution appeared which at a first order may be considered as independent on the temperature.

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