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Yield and plastic behavior of glassy polymers LUCA CONCA, Laboratoire Polymères et Matériaux Avancés, UMR 5268 CNRS/Solvay, ALAIN DEQUIDT, Institut de Chimie, Université de Clermont-Ferrand, DIDIER LONG, Laboratoire Polymères et Matériaux Avancés, UMR 5268 CNRS/Solvay, FRANÇOIS LEQUEUX, Physicochimie des Polymères et des Milieux Dispersés, ESPCI ParisTech, PAUL SOTTA, JEAN-YVES DELANNOY, Laboratoire Polyméres et Matériaux Avancés, UMR 5268 CNRS/Solvay — We extend here a model for the dynamics of non-polar polymers close to the glass transition, based on percolation of slow subunits. This model is solved in 3D by numerical simulations, in order to describe and calculate the mechanical properties of glassy polymers, from the linear regime up to the plastic regime of deformation, with a spatial resolution of 3-5 nm. We propose that the applied stress results in an acceleration of the dynamics of the subunits. Our simulations describe the onset of plastic behavior and the reorganization at the scale of dynamical heterogeneities. They allow for calculating how the relaxation time distribution is modified under applied stress. We show that deformation is localized in shear bands on the scale of about 10 nm at yield. Our simulation allow also for calculating the elastic and dissipative moduli as functions of strain amplitude and as functions of temperature. We show that G' decreases by several orders of magnitude at large deformation amplitudes as compared to the linear regime, whereas G'' decreases by a factor of about 3 only.

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