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Simulation of Large Deformation in Glassy Atactic Polypropylene

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A static, atomistic model has been used to study the stress-strain behavior of glassy, atactic polypropylene well beyond the yield point. The polymer is modelled as a single chain of carbon atoms with pendant hydrogen atoms and methyl groups, packed using a periodic parallelepiped continuation condition (initially an 18.5 Å cube) at a potential energy minimum. Deformation is simulated by imposing small strain steps on the periodic box, minimizing the system energy at the end of each step, which causes the polymer to seek a new conformation. Molecular movement can occur only by rotation around the skeletal C-C bonds; all bond lengths and angles are fixed.

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Pure shear and uniaxial extension strain increments were imposed on an ensemble of nine systems, to a total strain of 0.2. The system stress-strain curves for individual structures show a flat, reversible stress response at the initial stages of deformation, followed by a series of sawtooth-patterned elastic regimes separated by sharp stress drops due to major plastic relaxations. The elastic regions are reversible, while the plastic collapses are irreversible. Averaging the stress-strain curves for the ensemble smooths the information, showing an initial, elastic response, with a clear transition to plastic behavior. The yield point was at ≈ 0.05 strain, Von Mises stress ≈ 100 MPa. The average system pressure steadily increased, indicating a dilatant plastic response under the constant volume condition.

Atomic strains showed little relative motion in the chain during the reversible regions, and large relative motions over the entire system volume during the plastic collapse. From examinations of many stereo pairs of the changing polymer conformations during a plastic collapse, it is found that the whole chain moves in a complex way, the atomic rearrangement felt nearly uniformly throughout the length of the chain. The distribution of unit shear relaxations from the plastic strain collapses for the ensemble was found. The average plastic strain was $0.037 (\pm 0.035)$. If this transformation shear strain is taken to be typical for most vinyl glassy polymers, and this is compared with the results of strain rate change experiments, it is possible to estimate the sizes of the local volumes undergoing a unit plastic relaxation. From this we conclude that the local volumes undergoing a unit plastic relaxation must be much larger than previously conceived in earlier deformation models, and must be on the order of 40 to 60 Å on the side.

SIMULATION OF LARGE DEFORMATION IN GLASSY ATACTIC POLYPROPYLENE.

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A static, atomistic model has been used to study the stress-strain behavior of glassy, atactic polypropylene well beyond the yield point. The polymer is modelled as a single chain of carbon atoms with pendant hydrogen atoms and methyl groups, packed using a periodic parallelepiped continuation condition (initially an 18.15 Å cube) at a potential energy minimum. Deformation is simulated by imposing small strain steps on the periodic box, minimizing the system energy at the end of each step, which causes the polymer to seek a new conformation. Molecular movement can occur only by rotation around the skeletal C-C bonds; all bond lengths and angles are fixed.

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