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Molecular mechanism of viscoelasticity in aligned polyethylene ALI HAMMAD, HIKMATYAR HASAN, THOMAS SWINBURNE, Imperial College London, Dept. Physics, London SW7 2AZ, UK , STEFANO DEL ROSSO, LORENZO IANNUCCI, Imperial College London, Dept. Aeronautics, London SW7 2AZ, UK, ADRIAN SUTTON, Imperial College London, Dept. Physics, London SW7 2AZ, UK — Aligned polyethylene is used in industrial and medical applications due to its low density and high tensile strength. Extensive experimental work has been done to determine its mechanical properties, notably its viscoelasticity. However, the molecular processes that underlie these macroscopic properties are poorly understood. We develop a united atom model of aligned chains, in which intermolecular interactions are modelled by a Lennard-Jones potential, and the elastic energy within chains is modelled with harmonic springs. Using this simple model, we demonstrate the nucleation of solitons from chain ends, as one molecular chain is stretched with respect to another, and how load is transferred between chains in disregistry by intermolecular interactions. We develop an equation of motion for the movement of solitons along molecular chains, allowing us to replace a collection of aligned chains with a gas of solitons. Although solitons have been invoked to account for dielectric relaxation in crystalline regions of polyethylene, we believe this may be the first time they are discussed in the context of mechanical properties of aligned polyethylene.

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