

Abstract Submitted  
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**A Molecular Mechanism of viscoelasticity in aligned polyethylene**<sup>1</sup> A. HAMMAD, H. HASAN, T.D. SWINBURNE, M. KHAWAJA, Department of Physics, Imperial College London, London SW7 2AZ, S. DEL-ROSSO, L. IANNUCCI, Department of Aeronautics, Imperial College London, London SW7 2AZ, A.P. SUTTON, Department of Physics, Imperial College London, London SW7 2AZ — The key observed property of aligned polyethylene is its viscoelastic behaviour, which is traditionally fitted with Maxwell models [1]. Although these empirical models are successful at reproducing the mechanical response of the material, they fail to capture the underlying molecular mechanisms that lead to the observed viscoelastic behaviour. We explain the observed viscoelastic behaviour in terms of the formation, interaction and movement of solitons, and relate these molecular mechanisms to the semi-crystalline microstructure of the material. Using Molecular Dynamics we demonstrate the following results: (a) The formation of solitons from interfaces between crystalline and amorphous regions (b) The transfer of tensile load between molecular chains (c) the pile-up of solitons in a molecular chain that allows the concentration of stress at particular points (d) The disassociation of solitons into  $\pi$ -twistons at 300K.

[1] H Van der Werff and AJ Pennings. Tensile deformation of high strength and high modulus polyethylene fibers. *Colloid and polymer science*, 269(8):747–763, 1991.

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