Dynamic electrorheological response of nanorod polymer nanocomposites

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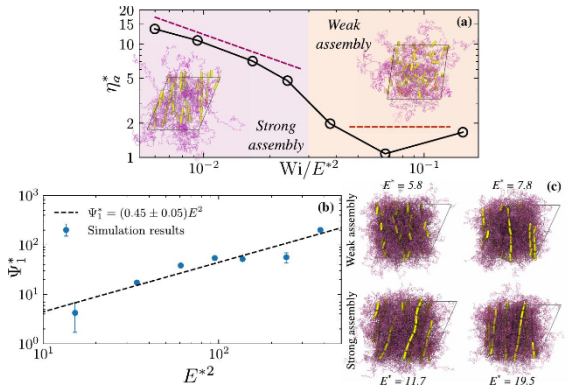
Smart materials, such as responsive polymer nanocomposites, are a type of functional materials capable of dynamically altering their macroscopic properties in response to external environmental stimuli, such as temperature, electromagnetic fields, pH, or salt concentration. For our investigation, we utilize a coarse-grained model in Langevin dynamics to unveil the interplay between the dynamical and rheological properties of a polymer matrix embedded with nano-sized polarizable rods under different electric fields of constant amplitude. Firstly, we test the transport properties of metallic nanorods and organic nanodimers in polyethylene without an electric field [1]. Then we study the collective behavior of a crowded environment of nanorods under an applied electric field [2]. Lastly, we investigate the introduction of nanorods with a 6.7% weight percentage concentration into a polymer matrix susceptible to an electric field [3]. Our results show structural motifs that scale with increasing field amplitude, affecting the steady-state dynamical and rheological properties, as well as the transitory electro-orientation response times. The nanorods structural transition goes through three phases: at low-fields we observe individual orientation but no collective behavior, at medium range fields we report filament formation, and at high amplitudes they self-assemble into percolating columnar structures. Our simulations under shear flow suggest that the structural phases of the nanorods directly affect the material's rheological properties, acting as a thickening agent that is enhanced with increasing field amplitude. At the highest tested field, we report a 15-fold increase in viscosity compared to the zero-field viscosity.

Keywords:
Polymer nanocomposites, Coarse-grained simulations, Molecular Dynamics, Electrorheology, Smart materials, Self-assembly, Conductivity, Nanorods



Response of (a) the low-shear apparent viscosity, (b) first normal stress coefficient, and (c) 4 snapshots at different electric fields.

References:

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Acknowledgements:
AP thanks grant no. PID2022-136540NB-I00 awarded by MICIU/AEI/10.13039/501100011033 and ERDF, a way of making Europe. DV, SEC and AP acknoweldge grant no. W911NF-23-1-0099 awarded by the U.S. Army Research Office. AMM thanks grant PID2023-149387OB-I00 awarded by MICIU/AEI/10.13039/501100011033 and FSE+ and grant C-EXP-187-UGR23 awarded by Consejería de Universidad, Investigación e Innovación and by ERDF Andalusia Program. All authors thank Servicio de Supercomputación UGR and PROTEUS, the supercomputing center of the Institute Carlos I for Theoretical and Computational Physics, for the computational time provided.