

Molecular dynamics simulations of Magneto-active elastomers

Author: Júlio P. A. Santos¹

Co-author: Sofia Kantorovich¹

¹ *Computational and Soft Matter Physics, University of Vienna, Austria*

Magneto-active elastomers (MAEs) [1-2], or magnetorheological elastomers, are composite materials whose properties - such as stiffness, surface roughness (wettability), and shape - can be controlled by low-energy magnetic fields, making them ideal for soft robotics.

MAEs consist of an elastic matrix embedded with magnetic micro- or nanoparticles, magnetically either hard (MH) or soft (MS). For high concentrations of particles, one can use a complex arrangement of springs that randomly bond nearby particles [3]. However, this model has oversimplified particle behavior (as permanent point dipoles) - critical for physically relevant MAEs.

We address this issue in ESPResSo [4], employing molecular dynamics to provide a critical comparison between MH- and MS-based MAEs. At zero field, MS particles do not interact magnetically, whereas MH particles form long chains within the layer. Increasing the field slowly promotes dipolar interactions between the MS particles and rapidly promotes Zeeman interactions with the applied field, leading to chains that aligned parallel to it. In contrast, MH chains must break before reorienting in the direction of the magnetic field, requiring larger applied fields for significant structural changes.

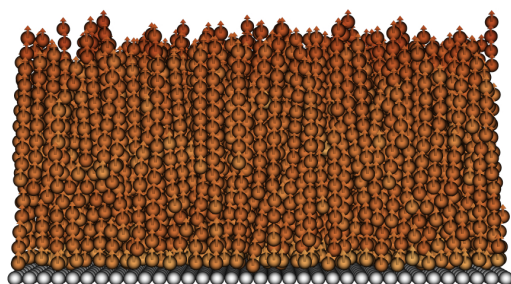


Figure 1: Simulation snapshot

Acknowledgements: This research is funded by the EU's Horizon Europe research and innovation programme Doctoral Network MAESTRI (grant agreement No. 101119614).

References

- [1] M. R. Jolly, J. D. Carlson, B. C. Muñoz and T. A. Bullions, *Intell. Mater. Syst. Struct.* 1996, 7, 613–622.
- [2] A. V. Chertovich, G. V. Stepanov, E. Y. Kramarenko and A. R. Khokhlov, *Macromol. Mater. Eng.*, 2010, 295.
- [3] P. Sánchez, E. Minina, S. Kantorovich and E. Kramarenko, *Soft Matter*, 2019, 15, 175–189.
- [4] F. Weik, R. Weeber, K. Szuttor, K. Breitsprecher, J. de Graaf, M. Kuron, J. Landsgesell, H. Menke, D. Sean and C. Holm, *The European Physical Journal Special Topics*, 2019, 227(14), (1789–1816).

Type:

Poster