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Toward a predictive model for elastomer seals. NICOLA MOLLINARI, MUSAB KHAWAJA, ADRIAN SUTTON, ARASH MOSTOFI, Department of Physics and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, UK — Nitrile butadiene rubber (NBR) and hydrogenated-NBR (HNBR) are widely used elastomers, especially as seals in oil and gas applications. During exposure to well-hole conditions, ingress of gases causes degradation of performance, including mechanical failure. We use computer simulations to investigate this problem at two different length and time-scales. First, we study the solubility of gases in the elastomer using a chemically-inspired description of HNBR based on the OPLS all-atom force-field. Starting with a model of NBR, C=C double bonds are saturated with either hydrogen or intramolecular cross-links, mimicking the hydrogenation of NBR to form HNBR. We validate against trends for the mass density and glass transition temperature for HNBR as a function of cross-link density, and for NBR as a function of the fraction of acrylonitrile in the copolymer. Second, we study mechanical behaviour using a coarse-grained model that overcomes some of the length and time-scale limitations of an all-atom approach. Nanoparticle fillers added to the elastomer matrix to enhance mechanical response are also included. Our initial focus is on understanding the mechanical properties at the elevated temperatures and pressures experienced in well-hole conditions.

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