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An atomistic model for cross-linked HNBR elastomers used in seals NICOLA MOLINARI, ADRIAN SUTTON, Imperial College London, Department of Physics, London SW7 2AZ, UK, JOHN STEVENS, Baker Hughes, Materials Centre of Excellence, Houston, Texas 77019-2118, USA, ARASH MOSTOFI, Imperial College London, Departments of Materials and Physics, London SW7 2AZ and the Thomas Young Centre for Theory and Simulation of Materials, UK — Hydrogenated nitrile butadiene rubber (HNBR) is one of the most common elastomeric materials used for seals in the oil and gas industry. These seals sometimes suffer "explosive decompression," a costly problem in which gases permeate a seal at the elevated temperatures and pressures pertaining in oil and gas wells, leading to rupture when the seal is brought back to the surface. The experimental evidence that HNBR and its unsaturated parent NBR have markedly different swelling properties suggests that cross-linking may occur during hydrogenation of NBR to produce HNBR. We have developed a code compatible with the LAMMPS molecular dynamics package to generate fully atomistic HNBR configurations by hydrogenating initial NBR structures. This can be done with any desired degree of cross-linking. The code uses a model of atomic interactions based on the OPLS-AA force-field. We present calculations of the dependence of a number of bulk properties on the degree of cross-linking. Using our atomistic representations of HNBR and NBR, we hope to develop a better molecular understanding of the mechanisms that result in explosive decompression.

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