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ATOMISTICALLY-INFORMED MACROSCALE POROSITY MODELS

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Abstract. Macroscale-derived porosity models might fail as pore size / ligament size approach the nanoscale. As an example, while the Hall-Petch law predicts an increase in strength as grain-size decreases, a breakdown in this law at the nanoscale has been observed. To make matters worse, many constitutive models do not take into account strain-rate effects, which are important in several extreme scenarios, like hypervelocity impact or shock wave studies. Atomistic molecular dynamics (MD) simulations of nanofoams subjected to high strain-rate compression do not compare well with continuum level simulations using standard constitutive models of porous materials, like the Gurson model. Several macroscale strain-based models will be compared amongst themselves and to the MD simulations, resulting in a new strain-based porosity model fit to nanoscale simulation results.