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Molecular dynamic modelling of fault rupture and crack dynamics

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We use a molecular dynamic based numerical model to investigate fault rupture and crack growth. In such a model complex global behaviour emerges from simple micromechanical rules of interaction between discrete elements in the model. These elements can be viewed as representing fundamental units of intact rock. We investigate how both fracture strength and toughness influence dynamic failure in both mode I and mode II, along preexisting faults (weak paths) in the model. In particular we focus on the factors which influence super shear wave rupture propagation for mode II cracks. For simple models, our results are in good agreement with predictions from analytical work. In more complex scenarios rich behaviour emerges, including dynamic stress triggering ahead of the crack tip. We also investigate crack growth into intact rock as the rupture reaches the ends of pre-existing faults. For mode I failures, crack acceleration is arrested through complex branching at the crack tips, maintaining a rupture velocity below the theoretical limit of the Rayleigh wave speed. For mode II, less complex wing-like cracks develop.