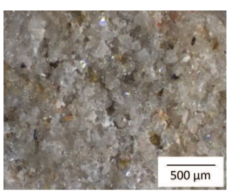
MESOSCALE MODELING OF QUARTZITE AND SANDSTONE UNDER SHOCK-LOADING AND HOMOGENIZATION TO MACROSCALE. N. Durr[1] and M. Sauer[1], [1]Fraunhofer EMI, Eckerstrasse 4, 79104 Freiburg, Germany, nathanael.durr@emi.fraunhofer.de

Introduction: In this contribution, we investigate the behavior of quartzite and sandstone under planar shock loading with numerical simulations on the mesoscale. These investigations are part of the MEMIN project [1], the intent is to generate a model that can be used to study small scale shock wave effects in sandstone and supplement material data for macroscale models. By using a planar shock wave, we reproduce in a simplified way the shock conditions a volume of rock material experiences from a meteorite impact. Quartzite is a compact aggregate of cemented quartz grains, the sandstone investigated here is characterized by a porosity of around 20 %. The mesoscale Finite Element model presented here includes intergranular interactions and porosity crushing under shock loading. The effects of porosity and quartz grain behavior on the macroscopic response are quantified via a homogenization approach.



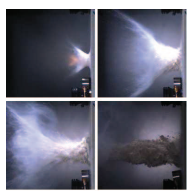


Fig. 1: Left:Micrograph view of a sandstone specimen. Right: Typical experiment from MEMIN: Sphere impact on a sandstone block at laboratory scale [2].

Mesoscale Material Model for Quartz:

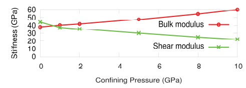
Equation of State. An appropriate Equation of State (EOS) able to represent highly shocked material is required. To this end, Quartz is modeled with a Mie-Grüneisen Equation of State, it accounts for compressibility variations as the confining pressure increases. The pressure P_{EOS} depends on internal energy e and density ρ using the following expressions:

$$P_{EOS} = P_H + \Gamma\rho(e - e_H) \quad \text{with } P_H = P_0 + \frac{\rho_0 {C_0}^2 \eta}{(1 - S\eta)^2},$$

$$e_H = e_0 + \frac{\eta}{\rho_0} P_H - \frac{\eta^2 {C_0}^2}{2(1 - S\eta)^2} \quad \text{and } \eta = 1 - \frac{\rho_0}{\rho}$$

where, for quartz, the Grüneisen Parameter $\Gamma = 0.9$, the bulk soundspeed is $C_0 = 3775$ m/s and $S = 1.695$. The bulk density of quartz is $\rho_0 = 2.65$ kg/m³ [3].

Elastic stiffness. In order to represent elastic stiffness, we use an elastic, pressure-dependent stiffness tensor of quartz that has been calculated using ab initio calculations of loadings in single lattice directions of crystals by Purton [4].

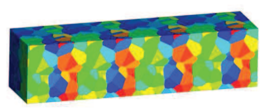


$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & 0 & C_{14} & C_{66} \end{pmatrix} \cdot \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{23} \\ \varepsilon_{31} \\ \varepsilon_{12} \end{pmatrix}$$

Fig. 2: Left: Pressure dependence of isotropic bulk and shear moduli of quartz (based on data from [4]). Right: Anisotropic stiffness matrix from which equivalent isotropic bulk and shear moduli were derived.

RVE geometry and boundary conditions:

RVE geometry. A Representative Volume Element (RVE) was generated. The grain size distribution is based on micrograph analysis, therefore, mesostructural stone properties such as grain arrangement or porosity are explicitly represented in the model. The average grain diameter used here is 100 µm. An RVE with a size of half a millimeter has about five grains per edge, this number is considered the minimum that is required to be representative for larger volumes. To get a stable pressure wave front in the simulation, a 2 mm-long row of four RVEs is assembled in the longitudinal direction.



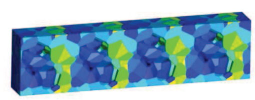


Fig. 3: Quartzite RVE (left) and longitudinal cut of sandstone RVE (right) created with the structure generator GEOSTAT.

Boundary conditions. A constant longitudinal velocity is applied to the left boundary of the RVE assembly at time zero. This boundary condition represents the shock wave produced by a projectile plate impacting the sandstone target plate in a planar plate impact experiment. Finite element nodes located on the RVE surfaces perpendicular to the prescribed velocity field are not allowed to move along the surface's normal direction in order to ensure a one-dimensional strain loading state.

Homogenization methodology: Using Homogenization, the locally observed mesoscopic quantities can be transferred into averaged macroscopic values. Here, the dependence of the shock wave speed U_S and the longitidunal compressive stress σ_{long} on the particle velocity U_p (both are interrelated through the Rankine-Hugoniot equations) are of interest, as this relation is required as input for a macroscopic EOS. In order to calculate macroscopic variables, a volumetric averaging of their local (mesoscopic) counterparts is carried out within the shocked region. Practically, the RVE is divided into several sub-volumes, in which an intermediate averaging is conducted.

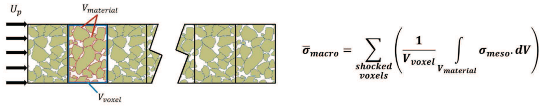


Fig. 3: Partitioning of a sandstone RVE into sub-volumes for homogenization purposes.

Mesoscale Simulations and Analysis:

Pore crushing in sandstone. Whether quartz grains exhibit a shear stiffness or not considerably influences the pore collapse in porous sandstone in the pressure range considered here. Two extreme cases are investigated: if the shear stiffness of quartz grains is zero, pores close quickly and the so-called jetting [5] takes place. In the case of quartz grains with shear stiffness, only moderate pore crushing (shrinking) occurs. Here, a longitudinal velocity of 1.5 km/s was applied.

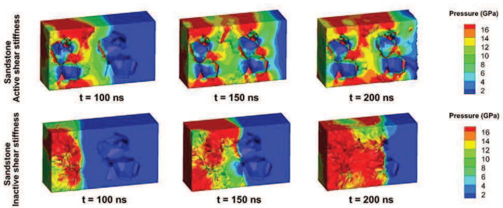


Fig. 4: Three snapshots of pressure contours in cross-sectional view of sandstone. Top: shear stiffness active. Bottom: shear stiffness inactive.

Macroscopic relationships for different quartz stiffnesses. Plots of U_S-U_P and σ_{long} - U_P relationships exhibit different features depending on the choice made on quartz stiffness and the type of rock considered. The pore crushing that occurs in sandstone slows wave propagation down and reduces macroscopic longitudinal stress compared to the same loading velocity in pure quartzite.

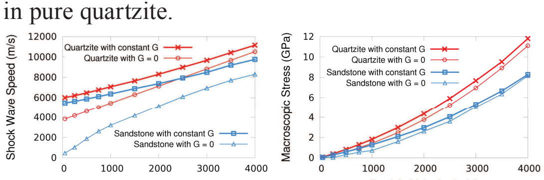


Fig. 5: Macroscopic U_S-U_P (left) and σ_{long} - U_P (right) relationships for quartzite and sandstone with constant and zero shear stiffness, respectively.

The pressure-dependent shear stiffness model leads to a slight decrease of the wave speed at intermediate particle velocities compared to the constant stiffness model. The high-velocity regime is dominated by hydrodynamic pressure, there, the influence of shear resistance is negligible.

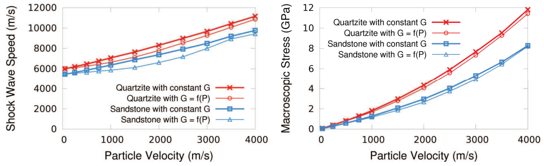


Fig. 6: Macroscopic U_S-U_P (left) and σ_{long} - U_P (right) relationships for quartzite and sandstone with constant and pressure-dependent shear stiffness, respectively.

In general, as far as porous materials are concerned, the increasing trend of the U_S-U_P curve is preceded by a first decrease until a global minimum is achieved. This minium typically occurs at lower velocities. For porous materials, this phenomenon originates from a flattening of the compressibility-density curve which occurs at the transition from the pure elastic to the shock loading regime. It is interesting to note that this feature has not been evidenced here, the reason is that the stiffness drop that occurs during pore crushing is not represented as plasticity and inter-/intragranular failure are not represented in the model. This effect is currently being investigated. Also, shock simulations with a closer-to-reality sandstone structure, which better represents grain boundaries and pore geometries, is ongoing. An example of such an improved mesoscale model is given in the following picture.

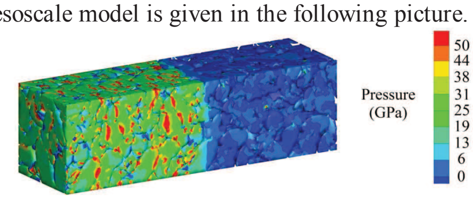


Fig. 7: Close-to-reality sandstone structure under shock loading. The applied longitudinal velocity is 1.5 km/s and contours indicate pressure.

References:

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