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A numerical study on mesoscale simulation of quartzite and sandstone under shock loading

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ABSTRACT

In this paper, we present two numerical models for the mesoscale (grain scale) simulation of planar shock waves in quartzite and sandstone using the in-house hydrocode SOPHIA. The models are compared in terms of their capability to represent physical mechanisms, such as phase transitions in quartz and pore collapse in sandstone, and they are validated by comparison to literature data. The study is part of the MEMIN (Multidisciplinary Experimental and Modeling Impact Research Network) project, which is devoted to the experimental and numerical investigation of the effects of meteorite impact on geological materials from laboratory scale to natural scale. The first model is based on the Smoothed Particle Hydrodynamics (SPH) method. Simulations with rather simplified structures in planar symmetry are presented. The model is used to investigate basic effects of porosity, pore geometry and water saturation. The second model presented is a more detailed, three-dimensional Finite Element (FE) model. With this model, the effects of grain anisotropy and different types of shear strength modeling are studied. In a parameter study, we investigate the influence of these parameters on shock Hugoniot relations, such as shock velocity (U_s) vs. particle velocity (U_p) and compressive longitudinal stress (σ_L) vs. U_p. Finally, the models are compared and the specific advantages and disadvantages of the different modeling variants are outlined.

1. Introduction

Meteorite impact on Earth is a wide topic that has gained more and more interest over the past years. This interest is motivated not only by the threat meteorites represent for human civilization, but also by the fact that some meteorites that collided with Earth millions of years ago can be traced back via the crater morphology they left behind. The crater morphology is influenced by the nature of soil meteorites strike. Meteorite material, size, impact speed and incident angle are key parameters for scientific investigations on meteorite impacts [1,2].

In the MEMIN (Multidisciplinary Experimental and Modeling Impact Research Network) project, geologic materials are investigated at laboratory scale through downscaled impacts of metallic spherical projectiles (up to one centimeter in diameter) onto quarried rock cubes (up to about half a meter edge length), see [3,4]. In the numerical parts of the MEMIN project, the mechanical behavior of those rocks is modeled at both mesoscale (grain scale) and macroscale. On the macroscale, a numerical rock model is typically validated by simulating impact experiments. The simulation methodology can then be extended to model meteorite impacts on Earth via the use of scaling laws [5]. The mesoscale modeling presented here is used to provide improved support for the material modeling in macroscale meteorite impact simulations. In general, macroscale models, which are based on continuum theory, need to be parameterized with material data. In the case of shock loading, this data is hard to find or generate and mostly restricted to measurements in simple one-dimensional loading conditions. For geologic materials, in particular, the variations of chemical composition, porosity, grain and pore size distributions, grain shapes, water saturation, pre-loading, etc. found in the field are very large, and it is not feasible to characterize the high rate behavior of each of these variants. For these reasons, mesoscale models can be very helpful and may improve macroscale material modeling. If the behavior of the constituents and their interaction is known and the model has been validated by comparison with experimental results, it can be modified and used to investigate the stress-strain relation for other material variants and for load cases which can hardly be generated experimentally, such as multiaxial dynamic loading. Following this approach, mesoscale models support the calibration of macroscale material models and improve the basis for extrapolations. Moreover, mesoscale modeling naturally supplies knowledge on shock wave effects on the microscale, such as grain fracturing and pore crushing [6], phase

Abbreviations: ANEOS, Analytical Equation of State; DEM, Discrete Element Method; FE, Finite Element; FV, Finite Volume; HEL, Hugoniot Elastic Limit; MEMIN, Multidisciplinary Experimental and Modeling Impact Research Network; PDF, Planar Deformation Feature; RVE, Representative Volume Element; SPH, Smoothed Particle Hydrodynamics

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Nomenclature

$\mathbf{1}$	Identity tensor (2nd order)
$\boldsymbol{A}$	Stiffness tensor coupling $\boldsymbol{S}$ and μ (2nd order)
$\boldsymbol{B}$	Stiffness tensor coupling P and $\varepsilon_{\boldsymbol{dev}}$ (2nd order)
$\mathbb{C}$	Isotropic elastic stiffness tensor (4th order)
$\mathbb{C}_{dev}$	Anisotropic deviatoric stiffness tensor (4th order)
e	Mass specific internal energy
e_H	Hugoniot energy
F	Free energy
G	Isotropic shear modulus
$\overline{G}$	Apparent shear modulus
G_{iso}^0	Equivalent isotropic shear modulus at zero pressure
$G_{iso}(P)$	Pressure-dependent equivalent isotropic shear modulus
G_{Reuss}	Lower Reuss bound for the equivalent isotropic shear modulus
G_{Voigt}	Higher Voigt bound for the equivalent isotropic shear modulus
K	Isotropic bulk modulus
K_{aniso}	Anisotropic bulk modulus
$\overline{K}_{EOS}$	Apparent bulk modulus prescribed by the Equation of State
K_{iso}^0	Equivalent isotropic bulk modulus at zero pressure
$K_{iso}(P)$	Pressure-dependent equivalent isotropic bulk modulus
K_{Reuss}	Lower Reuss bound for the equivalent isotropic bulk modulus
K_{Voigt}	Higher Voigt bound for the equivalent isotropic bulk modulus
m	Mass
m_{ref}	Reference mass
P	Pressure
P_H	Hugoniot pressure
$P_T(\rho)$	Isotherm pressure lines over density
$\boldsymbol{S}$	Deviatoric stress tensor (2nd order)
$\mathcal{S}$	Entropy
s	Linear coefficient of the U_s - U_p relationship
T	Temperature
$T_P(\rho)$	Isobar temperature lines over density
U_p	Particle velocity
$\overline{U}_p$	Average of U_p over m_{ref}
U_s	Shock velocity
V	Volume
V_{ref}	Reference volume
Y	von Mises yield stress
Γ	Grüneisen coefficient
ε	Infinitesimal strain tensor (2nd order)
ε_{dev}	Infinitesimal deviatoric strain tensor (2nd order)
μ	Compressive volumetric strain: $\mu = -\, tr(\varepsilon)$
ρ	Density
ρ_0	Initial density
σ	Cauchy stress tensor (2nd order)
σ_L	Compressive longitudinal stress under 1D strain conditions
$\overline{\sigma}_L$	Average of σ_L over V_{ref}

transitions and planar deformation features [7] and the influence of crystal anisotropies or grain boundaries [8].

Some features pertaining to the shock behavior of geological rocks have been already addressed in previous works. Pore crushing and grain fracturing have been modeled in [6] using a hybrid Smoothed Particle Hydrodynamics (SPH) and Discrete Element Method (DEM) formulation. However, since a two-dimensional geometry and a simple linear elastic model for quartz models have been employed, only a qualitative analysis could be provided. Quartzite and sandstone with idealized pore shapes using a Finite Volume (FV) approach have been investigated in [9]. Local pressure concentrations relatively to pore crushing and quartz phase transition effects could be predicted and quantified. Due to the use of idealized pore shapes, details such as grain shapes, boundaries and, in particular, crystallographic orientation, could not be explicitly modeled. Similar analyses have been conducted in [10] on generic granular materials. In order to capture geometries and realistic material properties in a unified way, two different Lagrange methods, namely the SPH method and the Finite Element (FE) method are employed in this work to capture compressive shock features in quartzite and sandstone on the mesoscale. For this purpose, the in-house hydrocode SOPHIA is used. Both methods are compared with each other and validated by literature on the basis of compiled shock data. The SPH method is applied to idealized material geometries with variable porosity and water saturation and shall, owing to its meshfree nature, capture extreme shock conditions in a convenient way. The model builds up on previous work in [9] and [11]. With the FE method, rather appropriate for lower shock conditions, we can reproduce more realistic geometries and investigate quartz shear strength effects on the macroscopic behavior of rocks. This model is an advanced version of the FE model presented in [12]. A parameter study is conducted in order to gain insight into pore collapse mechanics and to derive macroscopic shock Hugoniots from mesoscale quantities. The parameters varied are impact velocity, quartz shear strength, porosity and pore content. In particular, the evolution of shock velocity and compressive longitudinal stress or pressure against particle velocity will be assessed by recourse to homogenization techniques.

2. Experimental literature data on the shock properties of quartzite and sandstone

Shock conditions on geological materials are only sparsely addressed in the literature. Two main reasons can be put forward. First, the application of shock conditions at laboratory scale demands highly specialized and expensive equipment such as Planar-Plate Impact facilities. Such equipment is only available in a few laboratories worldwide. Secondly, most applications in shock physics concern military research, where metals and alloys are more widely investigated than geological materials or rocks.

Trunin et al. [13] present a large collection of shock data that has been gathered from the late 1940s to the end of 2000 by the All-Russian Research Institute of Experimental Physics. As far as quartzite and sandstone are concerned, shock Hugoniot relations such as shock velocity-particle velocity U_s - U_p relationships or pressure-density relationships can be found for silica SiO_2. The covered particle velocities range from 250 m/s to more than 20 000 m/s. Limited data for sandstone with different porosities is also available. Shipman et al. [14] present shock data inferred from shock wave loading on Coconino sandstone from a meteor crater in Arizona. The particle velocities and pressures achieved by their light gas gun facility range up to 6500 m/s and 14 GPa, respectively. Ahrens and Gregson [15] conducted shock experiments on a variety of crustal rocks by recourse to explosives. Shock data on Sioux quartzite, Eureka Quartz, Coconino Sandstone and Massilon Sandstone was obtained in a low shock regime, for which the particle velocity U_p does not exceed 2000 m/s.

Fig. 1 presents a collection of U_s - U_p data extracted from the aforementioned literature references for quartzite and sandstone. The lower shock regime, i.e. $U_p < 2000$ m/s, is separately focused on in Fig. 1-left in order to highlight the elastic-shock transition more properly. The complete data set is represented in Fig. 1-right. A