Stress field analysis in a stony meteorite under thermal fatigue and mechanical loadings

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\begin{abstract}
A micromechanical approach relying on 3D image-based finite element (FE) models, together with experimental testing, is employed to investigate the stress distribution in an L6 ordinary chondrite's microstructure subjected to thermal and mechanical loadings. An in-situ X-ray micro-computed tomography (micro-CT) setup capable of applying thermal and mechanical loads shed light on crack initiation mechanisms in chondrite samples. Micro-CT images were further used to reconstruct realistic microstructural models of the samples, which were transformed into FE models using an automated non-iterative mesh generation algorithm. FE approximation of stress fields showed that under mechanical loads, the stress often concentrates in matrix-particle interfacial regions with higher curvatures. This could result in the nucleation and eventually propagation of cracks in such regions. However, when the thermal cycling takes place, the stress concentrates more uniformly along with particle interfaces, resulting in their debonding from the surrounding matrix. Both observations were verified by experimental data obtained from in-situ micro-CT imaging.
\end{abstract}

1. Introduction

Identifying and quantifying stresses developed under mechanical loading (e.g., quasi-static and impact loads) or due to the thermal fatigue (e.g., diurnal thermally induced stresses) are important to further the current understanding about disaggregation of sitting rocks on the surface of airless bodies. Such knowledge has a direct implication in understanding regolith production and thus surface evolution of asteroids and their life expectancy. One of the main questions in this regard is to quantify the contribution of mechanical-induced stresses versus those caused by thermal fatigue on the asteroidal rock disaggregation. This requires understanding mechanisms associated with the crack initiation and coalescence, as well as the stress field associated with it in such environments.

Mechanical stresses caused by the collisional generation and micrometeorite impacts are widely regarded as the main mechanism that modifies the landscape surface of asteroids (Housen et al., 1979). During impact, the resultant kinetic energy is transferred by means of stress waves. While impact loads are compressive by nature, corresponding cracks often form due to a tensile stress regime emerged either by reflection of compressive waves from free surfaces or by displacement of the material outward from the impact site. Further, the impact not only influences the size distribution of surface materials but also leads to its spectral alteration by impact melt formation products (agglutinates) (Clark et al., 1992). Another point of consideration is that asteroids are relatively small to retain atmosphere (Housen et al., 1979) and are often classified as airless bodies. Thus, spatial and temporal changes in the temperature on the surface of asteroids can be significant. Severe thermal gradients on the surface could give rise to micro-cracking as a result of differential thermal expansion between constituent phases with different elastic moduli and thermal conductivities (Branner, 1895; Hazeli et al., 2018; Kranz, 1983). Despite the fact that the role of thermal fatigue on the formation of micro-cracks in rocks has extensively been studied, research on this topic in a planetary context is relatively new (e.g., Delbo et al., 2014, Hazeli et al., 2018, Molaro et al., 2015).

In the past century, the ability of thermal fatigue in breaking down surface rocks and boulders on Earth and other planetary bodies have been subjected to controversial debates. Recent studies based on field observations, laboratory experiments, and modeling, however, have confirmed the effectiveness of thermal fatigue on rock disaggregation on Earth, Mars, and airless bodies (Delbo et al., 2014; Dombard et al.,...
The surface temperature of asteroids follows a diurnal cycle with considerable temperature changes as the Sun rises or sets. Thermal stresses then arise from through-the-depth thermal gradients and the mismatch between coefficients of thermal expansion of cracks in constituent minerals. These thermally induced stresses can give rise to the initiation and propagation leading to rock breakdown. This process is known as thermal fatigue, and progressive thermal fatigue leads to thermal fragmentation (Kranz, 1983). Note that the magnitude of stresses themselves is not a direct indication that fracture will occur, because the fracture process is controlled by the asymptotic stress intensity factor at the crack tip (Ramesh et al., 2015).

Among previous studies, we can mention the semi-analytical framework developed in Delbo et al. (2014) to determine the stress intensity factor at the crack tip due to thermal fatigue and its impact on the fragmentation of surface rocks. A recent modeling effort introduced by Molaro et al. (2015) reported calculated grain-scale stresses induced by temperature variations in a mock stony meteorite microstructure. The calculations suggest that strongly heterogeneous stress distributions can arise during thermal cycling. More recently, Hazeli et al. (2018) conducted an integrated experimental study and 2D modeling effort focusing on crack propagation process as a result of thermal fatigue. This study showed that the primary fatigue crack path preferentially follows the interfaces between monominerals, leaving the minerals themselves intact after fragmentation. An experimentally informed, microstructure-based finite element analysis was then carried out to calculate the stress build up due to thermal fatigue (Hazeli et al., 2018).

It should be noted that the numerical studies cited in Molaro et al. (2015) and Hazeli et al. (2018) are limited to the two-dimensional (2D) space. Thus, the effect of the interaction between internal phases in a realistic 3D microstructure and corresponding stress concentrations along material interfaces are overlooked. Further, none of these studies consider the development and magnitude of internal stress as a result of the mechanical loading and only focus on the impact of thermal fatigue. In order to further advance these studies, in this work we experimentally investigate mechanisms of crack formation in a stony meteorite sample under mechanical loading and thermal fatigue in real time and in the three-dimensional space using X-ray micro-computed tomography. The experimentally collected tomography images are then employed to approximate the development of principal stresses in realistic, 3D microstructural models of the rock under quasi-static mechanical loadings. A comparison is also made between the distribution of stresses subject to mechanical loading versus thermal cycling. It is worth mentioning that although the current manuscript is only focused on analyzing the linear elastic response, it is the first study incorporating the realistic 3D microstructure of an asteroidal rock. Hence, it can shed light on damage initiation mechanisms in the rock but establishing more sophisticated models taking into account the nonlinear material behavior (damage growth, interfacial debonding) and strain rate (due to impact loading) would be necessary to fully capture the fragmentation process. Given the scarcity of asteroid samples and difficulties associated with experimental testing, proper calibration/validation of such models with actual material properties is a challenging task that demands more research in the field.

1.1. Recent significant observations

Images from Near-Earth Asteroid Rendezvous (NEAR) Shoemaker spacecraft from asteroid 433 Eros suggest a layer of loose sediment that blankets the entire asteroid surface, as shown in Fig. 1a–c (images courtesy of Dombard et al., 2010). It is suggested that the formation of sediment ponds could be attributed to the sitting boulder erosion by in-place mechanisms rather than the impact followed by seismic shaking that flattens the material into the pond morphology (Dombard et al., 2010, 2007).

A related case of interest pertains to images of comet 67P/Churyumov-Gerasimenko captured by the European Space Agency’s Rosetta spacecraft. The Rosetta lander, Philae, was equipped with an optical spectroscopic and infrared remote imaging system (OSIRIS) that acquired images of the surface at scales of < 0.8 m per pixel (Bibring et al., 2015; Thomas et al., 2015). OSIRIS observations suggested that surface features could be grouped into five categories: Dust-covered terrains (cf. Fig. 1d); brittle materials with pits and circular structures; large scale depressions; smooth terrains; and exposed consolidated surfaces. While it is stated that “the surface of comet 67P is almost devoid of recognizable impact craters”, several surprisingly large cracks are observed, including the 500 m long crack in the Anuket region and the 200 m long fracture in the Aker region (cf. Fig. 1e, courtesy of Thomas et al., 2015). The lack of concrete evidence of shear displacements along cracks and impact sites that might produce these cracks raises questions regarding mechanisms that govern the surface evolution (El-Maarry et al., 2015; Thomas et al., 2015). The fact that cometary (Thomas et al., 2015) and small asteroid (Delbo et al., 2014) surfaces are likely subjected to large temperature variations and temporal gradients could further raise doubt about the main cause of such cracks.

Another important observation was made by the NASA/Goddard Space Flight Center/GSFC/Arizona State University team. It recorded 20 m boulders fragmented at the end of their rolling track in an area around the craters Schiller, near the extreme southwestern limb of the Moon’s Earth-facing hemisphere. The fact that there is no impact evidence (e.g., crater or ejecta) suggests that the rock fragmentation could be the result of in-place erosion of boulders.

1.2. Surface modification mechanisms

Impacts evolve the surface of planetary bodies by creating craters and ejecting excavated materials. Studying the micrometeorite erosion of rocks on the Moon (the best analog available, cf. Fig. 2) suggests that 1 m of the rock can be eroded per 1 Gyr (Arvidson et al., 1975; Crozaz et al., 1971), which is too slow to supply the required material over the age of the Solar System (Dombard et al., 2010). Considering the fact that ejecta velocities for small kilometer-sized asteroids typically exceed the gravitational escape velocity Housen and Wilkening (1982), the amount of retained ejecta following a high-velocity impact event is highly limited. Images from the surface of the asteroid (25143) Itokawa, visited by the JAXA Hayabusa spacecraft, have revealed unexpectedly fine regolith on the Itokawa surface with no visible crater on the surface (Thomas et al., 2015). As noted above, the images taken by Rosetta lander (Philae) from comet 67P/Churyumov-Gerasimenko show the presence of considerably large surface cracks (El-Maarry et al., 2015), with no evidence of shear and impact. Therefore, mechanical stresses cannot be the only source of surface modification.

Surface modification has been also attributed to space weathering processes such as irradiation, implantation, solar wind sputtering (Noble et al., 2010; Pieters et al., 2000), and dielectric breakdown (Jordan et al., 2015). Similar to impact, space weathering can also change physical properties including optical spectra (Sasaki et al., 2015), as well as microstructural features such as the rock porosity (Tural, 2004). The lack of understanding about mechanisms involved in the surface rock break down and subsequent properties of surface materials could lead to the misinterpretation of remotely sensed data. Moreover, understanding physical and mechanical properties of regolith, which actively evolves with modification agents, is necessary to develop sampling methods for return missions. Understanding the stress distribution as a result of mechanical loadings versus thermal fatigue could potentially generate necessary knowledge about the size and distribution of fragmented rocks. Once one determines how the principal stresses build up under mechanical loadings and thermal fatigue, it would be possible to establish a correlation between the size and geometry of resultant fragments and the source of corresponding
stresses. This type of study could answer important questions such as the history and the source of surface evolution in samples retrieved from visited bodies.

1.3. Challenges and significance of 3D modeling

Several recent studies have pointed to the previously overlooked contribution of thermal fatigue to the landscape evolution of planetary bodies and in particular asteroids, e.g., Delbo et al. (2014), Dombard et al. (2010), Hazeli et al. (2018), Molaro et al. (2015), Pieters et al. (2000), and Robinson et al. (2001). Numerical analyses show that the thermal fragmentation induced by diurnal temperature variations breaks up rocks larger than a few centimeters faster than micrometeorite impacts (Delbo et al., 2014). It is reported that bodies rotating slowly close to the Sun have the largest daily temperature ranges, which leads to higher thermal-induced stresses. On the other hand, asteroids that are farther from the Sun have significantly smaller temperature ranges but rotate faster; thus experience a higher thermal cycling rate (Molaro et al., 2015). Understanding where in the solar system thermal fatigue breakdown may dominate requires studying damage mechanisms associated with the mechanical disruption versus the thermal fatigue on the surface of planetary bodies.

In general, one of the major challenges toward simulating the micromechanical behavior of rocks is to create realistic 3D models of their complex microstructure. In this study, we use high resolution X-ray micro-computed tomography (micro-CT) images to characterize the 3D heterostructure of an L6 ordinary chondrite. However, as will be discussed in Section 3.2, the complexity of microstructure and the lack of contrast between some constituents due to having similar densities lead to severe challenges during the processing and segmentation of the resulting imaging data. The microstructural model must then be converted to appropriate FE models to simulate the chondrite micro-
thermo-mechanical behavior. The main challenge here is to generate high-quality conforming (matching) meshes to discretize such complex geometrical models, as the quality of this mesh (i.e., elements shape and aspect ratio) has a direct impact on the fidelity of simulations. One could use various meshing algorithms for this purpose, among which we can mention the Delaunay triangulation (Shewchuk, 2002), advancing front (Lo, 1985; Schöberl, 1997), Quadtree/Octree techniques (Baehmann et al., 1987; Shephard and Georges, 1991), and Marching Cubes (Li and Zhang, 2014; Zhang et al., 2010). However, these algorithms rely on an iterative phase to improve element aspect ratios, which could be computationally demanding or even fail to converge for problems with complex geometries.

In the current study, we implement a non-iterative mesh generation algorithm coined Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) (Nagarajan and Sroghati, 2018; Sroghati et al., 2017a,b) to build high-fidelity FE models of an ordinary chondrite microstructure. A unique feature of CISAMR is the ability to non-iteratively transform a simple structured mesh composed of tetrahedral elements into a conforming mesh with proper element aspect ratios regardless of the complexity of the geometry. After the processing/segmentation of micro-CT images to characterize the asteroid’s microstructure and implementing CISAMR for mesh generation, resulting FE models are used to simulate the micromechanical behavior of the meteorite subject to thermal and mechanical loads. We have also compared resulting numerical simulations with in-situ micro-CT images of samples of this asteroidal rock under similar loading conditions. Approximated mechanical stresses in the chondrite microstructure are then analyzed to quantitatively understand damage initiation mechanisms for each type of loading.

2. Micromechanical model

2.1. Governing equations

Let \( \Omega \) be the macroscopic domain of an asteroidal rock with the boundary \( \partial \Omega = \Gamma \) and an outward unit normal vector \( \mathbf{n}_\Omega \). The domain boundary is divided into two non-overlapping regions, \( \Gamma = \Gamma_\text{e} \cup \Gamma_\text{n} \), corresponding to Dirichlet (prescribed displacements) and Neumann (applied traction) boundary conditions, respectively. At every point in the macroscopic coordinate system \( x_\Omega \) with a characteristic length of \( L \), we consider a microscopic domain \( \Theta \) with boundary \( \Lambda \) and an outward unit normal vector \( \mathbf{n}_\Theta \), which is described within the microscopic Cartesian coordinate system \( x_\Theta \). Note that the characteristic dimension \( l \) associated with \( \Theta \) must be significantly smaller than \( L \), i.e.,

\[
\xi = \frac{l}{L} \ll 1,
\]

where \( \xi \) is the ratio of the microscopic to macroscopic length scales. To correlate \( \Omega \) and \( \Theta \), we employ the first order asymptotic expansion theorem to decompose the displacement field \( u(x_\Theta, x_\Omega) \) emanating from thermo-mechanical loadings into macroscopic \( u_\Omega(x_\Omega) \) and microscopic \( u_\Theta(x_\Theta, x_\Omega) \) components as

\[
u \mathbf{u}_\Theta = \mathbf{u}_\Omega + \xi \mathbf{u}_n(x_\Theta, x_\Omega).
\]

Assuming the steady state heat conduction at both the macro and micro scales, the strong form of macroscopic thermoelastic governing equations is given by: Find \( \mathbf{u}_\Omega \) such that

\[
\begin{align*}
\nabla \sigma_\Omega &= 0 & \text{in} \Omega, \\
\sigma_\Omega &= C: \varepsilon_\Omega \quad & \text{in} \Omega, \\
\varepsilon_\Omega &= \frac{1}{2} (\nabla \mathbf{u}_\Omega + (\nabla \mathbf{u}_\Omega)^T) & \text{in} \Omega, \\
u \mathbf{u}_\Omega &= \mathbf{u}_n & \text{on} \Gamma_\text{n}, \\
\sigma_\Omega: \mathbf{n}_\Omega &= \mathbf{t} & \text{on} \Gamma_\text{e},
\end{align*}
\]

where \( C \) is the fourth-order elasticity tensor, and \( \sigma_\Omega \) and \( \varepsilon_\Omega \) are the macroscopic stress and strain tensors, respectively. As shown in this equation, \( \sigma_\Omega \) is composed of macroscopic mechanical strain \( \varepsilon_\Omega^m \) and thermal strain \( \varepsilon_\Omega^h \) terms, which are evaluated as

\[
\sigma_\Omega^m = \frac{1}{2} (\nabla \mathbf{u}_\Omega + (\nabla \mathbf{u}_\Omega)^T), \quad \sigma_\Omega^h = \varphi \Delta T.
\]

In the equation above, \( \varphi \) is the coefficients of thermal expansion (CTE) tensor and \( \Delta T \) is the change in temperature. The weak form of Eq. (3) can be written as: Find \( \mathbf{u}_\Omega \) such that

\[
\int_\Omega \sigma_\Omega: \mathbf{v}_\Omega \, d\Omega - \int_\Gamma_\text{e} \mathbf{t} \cdot \mathbf{v}_\Omega \, d\Gamma = 0 \quad \forall \, \mathbf{v}_\Omega \in \mathbf{V}_\Omega,
\]

where \( \mathbf{V}_\Omega \) is a sufficiently smooth function space defined as

\[
\mathbf{V}_\Omega = \{ \mathbf{v}_\Omega(x_\Omega) \mid \mathbf{v}_\Omega \in H^1(\Omega), \mathbf{v}_\Omega = 0 \text{ on } \Gamma_\text{n} \},
\]

with \( H^1(\cdot) \) being the first-order Hilbertian Sobolev space.

The equilibrium equation at the microscale is given by

\[
\nabla \sigma_\Theta = 0 \quad \text{in} \Theta,
\]

where \( \sigma_\Theta = C : \varepsilon_\Theta \) is the microscopic stress tensor that depends on \( \varepsilon_\Theta \) and the microscopic strain tensor \( \varepsilon_\Theta \). Defining free energy densities at macroscopic (\( \Phi_\Omega \)) and microscopic (\( \Phi_\Theta \)) scales as

\[
\Phi_\Omega = \frac{1}{2} \varepsilon_\Omega^m: \sigma_\Omega, \quad \Phi_\Theta = \frac{1}{2} (\varepsilon_\Theta + \varepsilon_\Omega^h): \sigma_\Theta - \epsilon \cdot \Theta \text{d} \Theta.
\]

The Hill-Mandel micro-homogeneity principle (Hill, 1985) can then be employed to correlate energy potentials at different scales as

\[
\inf_{\sigma_\Theta} \Phi_\Omega(\varepsilon_\Theta) = \inf_{\mathbf{u}_\Theta} \frac{1}{2} \int_\Theta \Phi_\Theta(\mathbf{u}_\Theta, \mathbf{u}_\Omega) \, d\Theta,
\]

where \( |\Theta| \) is the measure (volume in 3D) of \( \Theta \). One can use Eq. (9) to derive the weak form of governing equations at the microscale provided boundary conditions (BCs) imposed on \( \Lambda \) satisfy the strain averaging theorem, which can be expressed as

\[
\varepsilon_\Theta(x_\Theta) = \frac{1}{|\Theta|} \int_\Theta \varepsilon_\Omega(x_\Omega) \, d\Theta.
\]

Also, by applying standard variational principles to Eq. (9), the macroscopic stress tensor \( \sigma_\Omega \) can be evaluated as

\[
\sigma_\Omega = \frac{1}{|\Theta|} \int_\Theta \sigma_\Theta \, d\Theta.
\]

2.2. Boundary conditions

Various choices for BCs of the microscopic domain have been used in the literature, among which we can mention applied traction, applied displacement, and periodic BC (PBC). The latter is expressed as

\[
\mathbf{u}_\Theta = \mathbf{u}_\Omega = \mathbf{u}_n, \quad \mathbf{t}_n = \mathbf{t}_\Omega = \mathbf{t}_\text{n},
\]

where \( \Lambda_\text{e} \) and \( \Lambda_\text{n} \) are two parallel faces of \( \Theta \). It has been shown that PBC is one of the best options for performing micromechanical simulations by avoiding unrealistic stress concentrations and subsequently damage localization along macroscopic domain boundaries (Inglis et al., 2008; Terada et al., 2000). In this approach, a macroscopic stress or strain is applied to every point inside the domain rather than applying the load directly on boundaries. However, the implementation of PBC would not be feasible geometrical periodicity of the microstructural model. For heterogeneous materials, this feature can only be achieved by synthesizing the microstructure using an appropriate reconstruction algorithm (Yang et al., 2018), as the actual microstructure often lacks periodicity.

In this work, we aim to build FE models of the asteroidal rock directly based on micro-CT images, which does no yield a periodic microstructure and thus prohibits the use of PBC. The Minimal Kinematics BC (MKBC) (Mesarovic and Papadidi, 2005) is proposed as a viable alternative to PBC for modeling problems with non-periodic geometries. In MKBC, the macroscopic strain \( \varepsilon_\Omega \) is applied on domain boundaries in a weak sense, i.e.,
where indicial notations \((i,j)\) take values 1, 2, and 3. To prevent the rigid body rotation, six prescribed degrees of freedom (DOFs) must be constrained on three arbitrary points \((A, B, C)\) on \(\Lambda\) such that \(u_{m}^{A} = 0, u_{m}^{B} = 0, u_{m}^{C} = 0,\) and \(u_{m}^{C} = 0\). More details regarding the implementation of MKBC are presented in Inglis et al. (2008), which also provides a quantitative comparison between its performance versus PBC.

Applying the weak form of macroscopic strains using Eq. (13) in MKBC avoids unrealistic stress concentrations along domain boundaries. However, its implementation introduces additional constraints on the displacement field to satisfy the macroscopic strain, which significantly increases the condition number of the stiffness matrix. Note that it would not be feasible to use an iterative solver to approximate the field when the stiffness matrix is severely ill-posed. Instead, one can implement a direct solver (Mesarovic and Padbidri, 2005) and the Lagrange multipliers (Inglis et al., 2008) to solve the augmented system formed by MKBC and impose the macroscopic strains on domain boundaries, respectively. However, for problems with a high number of DOFs, even after applying pre-conditioners and using parallel computing, a direct solver may not be capable of handling the resulting ill-conditioned system of equations. We faced this challenge when attempted to utilize MKBC in this work: Regardless of the computing capacity (up to 1000 processors), it was not feasible to perform a thermoelastic simulation on FE models of the chondrite microstructure (> 3 million DOFs) using any of the direct solvers available in the PETSc C++ library (http://www.mcs.anl.gov/petsc).

Given the limitations of PBC and MKBC outlined above in the context of the current study, we employ mixed prescribed displacement and traction free BCs to simulate the micromechanical behavior of the meteorite. A drawback associated with using such BCs is the development of unrealistic stress concentrations near domain boundaries, which must be discarded while analyzing results. For the FE models of the chondrite microstructure (cf. Section 3.3), this undesirable effect is limited to a thin layer along each boundary. Thus, after performing each simulation, we simply chop off the elements falling in these layers from all faces of the domain and only analyze realistic stresses developed within the interior region.

3. Image-based modeling process

3.1. In situ micro-CT data acquisition

As noted previously, we aim to analyze the stress distribution in an L6 ordinary chondrite (GRO 85209) subject to both thermal and mechanical loads. Two optical images of the surface of this meteorite are illustrated in Fig. 3a and b, which consists of Fe-Ni and chondrule particles embedded in a mineral matrix composed of plagioclase and mafic. Fig. 3c shows a 2D slice of the corresponding micro-CT imaging data, which was acquired at the beamline 8.3.2 in the Advanced Light Source facility located in Lawrence Berkeley National Laboratory. The samples utilized for the in-situ mechanical and thermal tests were cut into cubes with the length 5 mm using a diamond saw. The X-ray CT system was operated in polychromatic mode centered on 40 keV with an exposure time of 100 ms for each of the 1025 projections, with a complete 360° rotation. Each projection was 2560 × 1488 pixels with a resolution of approximately 3.2 μm. More details on this X-ray CT system and its data acquisition parameters are presented in MacDowell et al. (2012). The transmission data from each projection was then converted to attenuation radiographs and reconstructed using the Livermore Tomography Tools (LTT) (Champley, 2016) reconstruction package, which implemented a parallel beam filtered back projection and an offset detector (i.e., half-scan) reconstruction algorithm. Note that, while Fe-Ni particles are clearly visible in the micro-CT data (cf. light gray color in Fig. 3c), it is extremely difficult to distinguish chondrule inclusions from the surrounding matrix due to their low contrast.

In addition to micro-CT scanning of the chondrite sample in its undeformed state, an in-situ micro-CT setup was utilized to extract the information associated with damage mechanisms under mechanical loading and thermal fatigue. The in-situ mechanical loading setup consists of a loading stage developed by Haboub et al. (2014) and Bale et al. (2013), as shown in Fig. 4a. This mechanical testing device performed under uniaxial, quasi-static compression mode using two platens at a rate of 5 μm/s, under a displacement-controlled condition. A total of 8 micro-CT scanning measurements at different load increments were recorded using the same scanning parameters as the unloaded sample, which resulted in an average scanning time of 8 to 10 min while the compression load was held constant. The maximum load during the test was 1580 N, at which the sample was considerably damaged.

The thermal fatigue setup was performed using a hot plate and a thin layer of adhesive tape to prevent any motion of the sample during the micro-CT scanning process. The temperature was monitored and recorded on the hot plate using a thermistor. Fig. 4b illustrates the sample mount and the hot plate setup for applying a cyclic thermal load. The sample was subjected to a 20 °C/min thermal rate for 47 heating-cooling cycles between 50 °C and 200 °C. Due to conductive and convective properties of the sample, the heating section of the cycle took on average 8 min to reach the peak temperature, while the cooling period required 13 min. The sample was scanned at room temperature, at 50 °C, and at 200 °C during the first cycle and at the end of the test.

It is worth mentioning that the thermal loading rate adopted in this work (i.e., 20 °C/min) is higher than what typically sustained by
characteristics. If the di-material phases in the imaging data depends on their X-ray absorption properly identi-son the test at a lower rate was simply unfeasible. As noted previously, the main goal of the numerical simulations presented in this manuscript is to quantify damage initiation mechanisms by analyzing the mechanical stresses developed in the rock due to thermal and mechanical loadings.

3.2. Microstructure reconstruction

While micro-CT is a powerful non-destructive tool for visualizing microstructural features (Seeram, 2015), the contrast between different material phases in the imaging data depends on their X-ray absorption characteristics. If the difference between densities of two phases (in this case, chondrule inclusions and the matrix) is not significant, they absorb similar levels of X-ray and a poor contrast appears between them in recorded radiographs. However, since the difference between thermoelastic properties of the chondrule and those of the matrix cannot be overlooked during the stress analysis, this lack of contrast is a major challenge for realistic reconstruction of the microstructure. Fig. 5a illustrates a statistical volume element (SVE) of the meteorite sample directly reconstructed based on its micro-CT data after applying appropriate image processing steps (i.e., noise filtration, smoothing, and segmentation; Sonka et al., 2014). As expected, only the Fe-Ni phase is identified and there is no trace of chondrule inclusions in segmented data. Thus, creating a realistic SVE requires virtually adding chondrule particles to the original model created via a direct reconstruction approach.

Although embedded chondrule inclusions in the GRO 85209 meteorite sample cannot be identified after image processing, it would be feasible to distinguish interfaces between these inclusions and the surrounding matrix in the micro-CT data by visual inspection. As shown in Fig. 5b, one can visually identify 2D cross-sectional geometries of

chondrule particles in multiple slices of micro-CT images. Here, we characterize the shape of each cross-section using a closed Non-Uniform Rational B-Splines (NURBS) curve. NURBS are parametric functions composed of B-Splines that are interpolated on a set of control points (Piegl and Tiller, 2012). In order to facilitate the characterization of the 3D morphology of each chondrule particle, the same number of control points are used to create NURBS curves representing its cross-sections on different stacks of micro-CT slices. As depicted in Fig. 5b, these NURBS curves are then extruded in the direction perpendicular to these slices to generate a 3D NURBS surface representing the particle morphology. Next, the resulting NURBS parameterization of each particle is added to the model directly reconstructed from micro-CT data (cf. Fig. 5a) to build the final SVE. As shown in Fig. 6, we have employed this approach to create two distinct SVEs corresponding to different regions of the chondrite sample.

3.3. Automated mesh generation

The next step is to transform the ordinary chondrite SVEs shown in Fig. 6 into high-fidelity FE models to accurately approximate the micromechanical stresses caused by thermal and mechanical loadings. This in turn requires the construction of high-quality conforming meshes with proper element shapes and aspect ratios, as well as a negligible geometric discretization error along material interfaces. As noted previously, in this work we implement the CISAMR algorithm (Nagarajan and Soghrati, 2018; Soghrati et al., 2017a) for mesh generation. The non-iterative process of transforming a structured tetrahedral mesh into a conforming mesh in CISAMR is depicted in Fig. 7, which involves four major steps: (i) h-adaptive refinement along material interfaces to reduce the geometric discretization error and more accurately recover stress concentrations in such regions; (ii) r-adaptiveivity of the nodes of elements cut by material interfaces, during which some nodes are snapped to nearby interfaces. On average, 50% of initially nonconforming tetrahedrons are transformed into conforming elements after the completion of this step; (iii) face-swapping to eliminate a small number of excessively deformed tetrahedrons with high aspect ratios, which emerge due to specific node-relocation patterns during the r-adaptivity phase; (iv) sub-tetrahedralizing the remaining nonconforming elements using certain rules for cutting their faces to build the final conforming mesh. CISAMR ensures that the aspect ratio

asteroidal rocks in actual case scenarios. It is understood that the heating/cooling rate is one of the dominant factors in the initiation and growth of damage in rocks, e.g., a rate lower than 2 °C/min often does not cause considerable cracking. Therefore, while the thermal rate of 20 °C/min leads to significant cracking in a few number of cycles, a much higher number of cycles would be required at lower heating/cooling rates to cause a similar damage density. Note that the high thermal rate of 20 °C/min is only applied during the in-situ experimental testing due to practical concerns, as a prolonged continuous access (e.g., several weeks or months) to the micro-CT device to perform the test at a lower rate was simply unfeasible. As noted previously, the main goal of the numerical simulations presented in this manuscript is to quantify damage initiation mechanisms by analyzing the mechanical stresses developed in the rock due to thermal and mechanical loadings.

Fig. 4. (a) Mechanical testing setup for compression loading; (b) thermal cycling setup via in-situ micro-CT.
of resulting elements does not exceed 5, although for majority of them this value is less than 3. More algorithmic details regarding this method are presented in Nagarajan and Soghrati (2018).

Fig. 8 shows portions of the conforming mesh generated using CI-SAMR for discretizing SVE 1 (Fig. 6a). A cubic structured mesh composed of 70 blocks of tetrahedrons along each edge (more than 1.71 million elements) is used as the background mesh for discretizing this microstructure. Depending on the size, curvature, and close proximity of particles, either one or two-levels of $h$-adaptive refinement is applied to background tetrahedrons adjacent to material interfaces. The total number of elements in the final conforming mesh is more than 4.85 million, which corresponds to 3.19 million DOFs in the FE model.

4. Results and discussions

FE models of the ordinary chondrite SVEs shown in Fig. 6 are employed to simulate their micromechanical response subject to compressive, shear, and thermal loads. The resulting maximum principal stress field in the mineral matrix and the von Mises stress field in Fe-Ni particles are adopted as precursors for the initiation of damage in each phase. Under a compressive load, mixed prescribed displacement and traction-free BCs are applied along domain boundaries in FE models. In these simulations, the bottom face of SVE is constrained against $z$-displacement ($u_z|_{L_{z}} = 0 \, \mu m$), while a constant displacement jump of $u_z|_{L_{z}} = -0.15 \, \mu m$ is applied to nodes on the upper face. In order to replicate a pure macroscopic shear strain, the following displacement BCs are prescribed on faces with $\pm n_x$ and $\pm n_z$ outward normal vectors: $u_x|_{L_{z}} = 0.15 \, \mu m$, $u_z|_{L_{z}} = -0.15 \, \mu m$, $u_x|_{L_{z}} = 0.15 \, \mu m$, and $u_z|_{L_{z}} = -0.15 \, \mu m$. Under a thermal loading, which is assumed as a uniform temperature rise of $\Delta T = 15 \, ^{\circ}C$, six DOFs at three corners of the domain are constrained to prevent rigid body motions. It is worth mentioning that typical mechanical and thermal loads applied to an asteroidal rock are often much higher than those assumed above (e.g., thermal loads could be up to 10 times higher). However, given the assumption of linear elastic material behavior in the FE analyses presented next, resulting stresses are linearly scalable and these loadings are selected to ensure that plastic deformations in Fe-Ni particles and cracking in the mineral matrix are negligible. In other words, these simulations are intended to shed light on damage initiation mechanisms in each SVE rather than predicting the evolution of damage.

As noted previously, applying either Dirichlet BC or Neumann BC leads to unrealistic stress concentrations along domain boundaries in the resulting simulations. To eliminate this effect, a thin layer with the thickness 32 $\mu m$ (equivalent to two layers of elements of the background mesh) is chopped off from all six faces of SVE before analyzing the recovered stress field. A numerical study showed that this approach...
Fig. 7. Non-iterative process of transforming a structured mesh into a high-quality conforming mesh using CISAMR.

eliminates all elements with an unrealistic stress recovery due to boundary effects without discarding a large volume of the domain originally simulated. Thermal and mechanical properties used for meteorite’s constituents are presented in Table 1 (Hazeli et al., 2018).

Figs. 9 and 10 illustrate FE approximations of the maximum principal stress $\sigma_{\text{max}}$ in SVE matrices under compressive and shear loads, respectively. The stress field in a slice of the domain parallel to the xy-plane (shown with dashed lines) is also depicted in each figure. According to these simulations, $\sigma_{\text{max}}$ is highly concentrated along interfaces with Fe-Ni particles, with a significant variation due to their changes in the curvature of the interface, as well as relative distances between particles. Note that despite applying a compressive load, several sites with tensile principal stresses are observed in the matrix, which could cause the crack nucleation in the semi-brittle mineral matrix. A more meticulous look at Figs. 9 and 10 reveals that peaks of stress concentration occur in regions where two or more Fe-Ni particles are in close proximity, re-emphasizing the importance of realistically incorporating the meteorite microstructure in the FE model. It is worth mentioning that the lower curvature of chondrule inclusions compared to Fe-Ni particles, together with a smaller difference between their elastic modulus with that of the matrix (cf. Table 1), leads to smaller values of $\sigma_{\text{max}}$ along their interfaces. 2D slices of $\sigma_{\text{max}}$ in Figs. 9 and 10 clearly show that principal stress concentrations in the matrix are higher along Fe-Ni particle compared to chondrule inclusions.

In-situ imaging results from the compression test described in Section 3.2 are depicted in Fig. 11. Although the sample did not fail at 1580 N, crack nucleation and propagation in the matrix emerged while the sample was being loaded. Similar to the FE simulations, the micro-CT slices through the volume shown in Fig. 11b indicate that sites with a high density of Fe-Ni particles are more prone to crack initiation. Fig. 11c, which corresponds to oval-shaped regions marked in Fig. 11b, shows the nucleation of cracks in the matrix along its interface with regions of higher curvature on Fe-Ni particles. This behavior is compatible with sites of high stress concentrations predicted by the FE model. Further, the deformed state of the matrix in the test shows crack extension and propagation through the matrix in regions more heavily populated with Fe-Ni particles. Note that although in the linear elastic simulations presented in this work we have not incorporated the weak interfacial bonding along material interfaces (e.g., via cohesive elements), it is expected that initially the damage occurs in the form of particle-matrix debonding due to the concentration of principal tensile stresses. Because such stress concentrations are further magnified in the matrix after debonding, the damage mechanism transforms into crack nucleation in this phase.

FE approximations of $\sigma_{\text{max}}$ in the matrix of the ordinary chondrite SVEs subject to a thermal load of $\Delta T = 15$ °C are illustrated in Fig. 12. Similar to the simulations performed under compressive and shear loads, $\sigma_{\text{max}}$ is highly concentrated in the vicinity of Fe-Ni particles. However, in this case, stress concentrations are more uniformly distributed along their interfaces with the surrounding matrix. This observation is verified by experimental results shown in Fig. 13, where applying a thermal fatigue load initially leads to interfacial damage (debonding) along a large portion of Fe-Ni particle surfaces rather than crack initiation in the matrix, which occurred under mechanical loading. The experimental results presented in Fig. 13c indicate that after 47 cycles of heating-cooling between 23 °C and 200 °C, the low strength of the matrix eventually causes the nucleation and propagation of cracks in this phase. However, this crack propagation is an artifact of debonding of Fe-Ni particles from the matrix, which magnifies stress concentrations in the latter along debonded regions.

It is also worthwhile to compare the maximum principal stress values $\sigma_{\text{max}}$ obtained from current simulations versus those reported in Hazeli et al. (2018) and Molaro et al. (2015). Although the former reference attempts at taking into account the actual shape of embedded particles, both studies rely on 2D FE models that cannot incorporate the realistic microstructure of a rock. Further, applied boundary conditions in these works are not identical to those adopted for the 3D simulations presented in this work. In Hazeli et al. (2018), the estimated maximum principal stress under a thermal loading of $\Delta T = 100$ °C in the same asteroidal rock as that studied here is 260 MPa. Note that material properties used for the ordinary chondrite constituents in the present study are identical to those reported in that reference. Given the assumption of linear elastic material behavior, linearly scaling up the resulting $\sigma_{\text{max}}$ values for $\Delta T = 100$ °C yields $\sigma_{\text{max}} = 285$ MPa and 373 MPa for SVE 1 and SVE 2, respectively. This shows that the 2D plane stress model used in Hazeli et al. (2018) under-estimates $\sigma_{\text{max}}$.
values, which is an expected outcome due to the higher curvature of inclusions in the 3D SVEs studied here.

For the transient 2D model considering circular-shaped inclusions in Molaro et al. (2015), the case with a negligible temporal temperature change, i.e., before the sunrise at one solar day, can be used as the point of comparison. The corresponding magnitude of $\sigma_{\text{max}}$ reported in this reference is $\approx 150 \text{ MPa}$, which is much lower than those predicted by the 3D FE models in this manuscript. However, in addition to significant difference in the curvature of inclusions in the two models, the model presented in Molaro et al. (2015) considers a higher elastic modulus and a twice larger coefficient of thermal expansion for the matrix, which makes a one to one comparison more difficult. It must be emphasized that the present study mainly aims at analyzing the distribution (and not magnitude) of $\sigma_{\text{max}}$ in the matrix to quantify the damage initiation mechanisms in the chondrite, as the magnitude of $\sigma_{\text{max}}$ does not proportionally change by increasing the loading due to the nucleation and growth of damage.

A comparison between distributions of $\sigma_{\text{max}}$ in a subdomain of SVE 1 under different loading conditions is presented in Fig. 14. As shown in this figure, applying compressive and shear loads leads to distinct locations for peak values of $\sigma_{\text{max}}$, which depend on both the curvature of the interface and the type of loading. As noted previously, $\sigma_{\text{max}}$ has a more uniform distribution along Fe-Ni interfaces subject to a thermal load, which is more clearly illustrated in Fig. 13c. This indicates that a large interfacial region between the matrix and Fe-Ni particle could be simultaneously debonded under this type of loading; a behavior that was also observed experimentally.

Finally, approximated von Mises stress fields ($\sigma_{\text{VM}}$) in Fe-Ni particles of SVE 1 subject to shear, compressive, and thermal loads are illustrated in Fig. 15. Given the ductile behavior of Fe-Ni, $\sigma_{\text{VM}}$ can be used as a
precursor for the initiation of plastic deformations and eventually damage nucleation in this phase. As shown in Fig. 15, a significant resemblance is observed between simulation results under compressive and thermal loadings. Further, for all types of loadings, peak values of $\sigma_{VM}$ occur in regions of high curvature on the surface of the largest particle. Such sites of stress concentration have a considerably higher value compared to the peak value of $\sigma_{max}$ in the matrix. As verified by in-situ testing, the lower strength of the mineral matrix compared to the Fe-Ni phase leads to the accumulation of damage and eventually the breakdown of the former before the nucleation of damage in Fe-Ni particles. However, high values of $\sigma_{VM}$ in high curvature regions of Fe-Ni particles indicate the possibility of localized plastic deformation in these particles. Note that the simulations presented in this work are based on the assumption of linear elastic behavior of all constituents,

Fig. 9. FE approximation of the maximum principal stress field in the mineral matrix of (a) SVE 1 and (b) SVE 2 subject to a compressive load.

Fig. 10. FE approximation of the maximum principal stress field in the mineral matrix of (a) SVE 1 and (b) SVE 2 subject to a shear load.
**Fig. 11.** (a) 3D rendered micro-CT volume of the meteorite sample used in the compression test; (b) two slices of CT images at 1.41 mm and 2.6 mm from the top of the sample; (c) enlarges views of subdomains of slices depicted in figure b, showing the formation of cracks subject to a 1580 N compressive load.

**Fig. 12.** FE approximation of the maximum principal stress field in the mineral matrix of (a) SVE 1 and (b) SVE 2 subject to the thermal load $\Delta T = 15$ °C.
which cannot capture this behavior.

5. Conclusion

A combination of high-fidelity FE modeling and in-situ micro-CT imaging during experimental testing was employed to investigate the micromechanical behavior of an L6 ordinary chondrite sample under mechanical and thermal loadings. Micro-CT images of the sample were processed to build two distinct microstructural models, which were subsequently converted into high-quality conforming meshes using a non-iterative meshing algorithm. FE simulations were carried out to analyze stress fields in the meteorite microstructure under shear, compressive, and thermal loads. Main takeaways from this study, which were verified experimentally via in-situ micro-CT imaging, are summarized below:

- Under mechanical loading, the maximum principal stress in the matrix is highly concentrated in regions with highest curvatures along Fe-Ni particle surfaces, which could eventually lead to the nucleation and growth of cracks in such regions. These sites of stress concentration are often different under shear and compressive loads but their magnitudes are considerably larger than stress concentrations along chondrule inclusions. This observation indicates that cracks initiate in the matrix due to the high tensile principal stresses...
in high curvature interfacial regions along Fe-Ni particles, in particular when these particles are in close proximity.

- Under thermal cycling, stress concentrations are more uniformly distributed along inclusion-matrix interfaces, with a higher concentration in the vicinity of Fe-Ni particles. This stress distribution indicates that interfacial debonding is the more likely damage mechanism when the meteorite is subjected to thermal fatigue. The debonding of the matrix from embedded inclusions magnifies stress concentrations in the former, which eventually leads to the initiation and propagation of cracks.

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