A nonlinear and time-dependent visco-elasto-plastic rheology model for studying shock-physics phenomena

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Abstract
We present a simple and efficient implementation of a viscous creep rheology based on diffusion creep, dislocation creep, and the Peierls mechanism in conjunction with an elasto-plastic rheology model into a shock-physics code, the iSALE impact code. Our approach is based on the calculation of an “effective viscosity” which is then used as a reference viscosity for any underlying viscoelastic (or even visco-elasto-plastic) model. Here we use a Maxwell-model which best describes stress relaxation and is therefore likely most important for the formation of large meteorite impact basins. While common viscoelastic behavior during mantle convection or other slow geodynamic or geological processes is mostly controlled by diffusion and dislocation creep, we show that the Peierls mechanism dominates at the large strain rates that typically occur during meteorite impacts. Thus, the resulting visco-elasto-plastic rheology allows implementation of a more realistic mantle behavior in computer simulations, especially for those dealing with large meteorite impacts. The approach shown here opens the way to more faithful simulations of large impact basin formation, especially in elucidating the physics behind the formation of the external fault rings characteristic of large lunar basins.

KEYWORDS
hydrocodes, impact cratering, iSALE, visco-elasto-plastic rheology

1 | INTRODUCTION

The viscoelastic behavior of material has been studied intensively over the last decades. Studies range from engineering and industrial applications,1-4 as well as biological,5,6 medical,7-9 and geological objectives.10-14 The concept of viscoelasticity was first proposed by Maxwell in 1867.15 Later on, progress in the understanding of crystal structures of geological
materials resulted in improved mathematical and physical models, such as the diffusion creep model or a power-law dislocation creep model. These and other improvements to the description of viscoelastic behavior contributed to a better understanding of (geo)dynamical problems, such as plate tectonics, mantle convection, mountain ridge formation, or dynamic earthquake ruptures. Over the last decades, extensive efforts have been made to develop and improve numerical rheology models to further increase the realism of numerical simulations.

It is widely known that the viscous rheologic properties of the mantle material have a significant effect on tectonic processes, such as subduction, folding, mountain formation, and even the growth of fractures and faults. It has also been established that extremely large meteorite impacts could have induced significant deformation of the Earth’s mantle during the Hadean era of heavy meteorite bombardment. However, most previous numerical simulations failed to include a proper model for the viscous deformation of mantle material. In contrast to many other geodynamical applications, where both the timescales and the length scales are long (up to millions of years for the formation of mountains), meteorite impact is a very rapid process with relevant timescales ranging from milliseconds to seconds and strains many times larger than 100%. Thus, it is plausible that small-scale phenomena occurring under high deviatoric stresses, such as changes in the crystal lattice, might become important in describing the macroscopic effect of viscoelasticity during impact processes. Furthermore, meteorite impacts generate shock waves (compressive waves) that propagate with speeds higher than the sound speed in the surrounding material. Irreversible compression and adiabatic decompression of the material occur, resulting in different types of shock effects (such as vaporization, melting fracture, collapse or opening of pore spaces), depending on the structure of the shock wave and the subsequent rarefaction wave. Some authors argue that the viscosity of geologic materials might be able to initiate a rate-dependent energy dissipation mechanism (often identified as a “shock viscosity”) that can broaden the shock wave and therefore might change the resulting shock effects. Stewart argued that incorporation of viscosity in the mantle of the Moon underlying the Orientale basin might have suppressed the excavation of mantle material onto the surface. However, lacking a proper visco-elasto-plastic rheology model for shock-physics codes, this has not been carefully tested. Here, we present our implementation of such a rheology into the shock-physics code iSALE.

High-stress rheology may play a particularly important role in the collapse of very large craters, such as the lunar basins or the Chicxulub crater on Earth. The impact of a large asteroid initially opens a large and deep transient crater that may be thousands of kilometers wide and hundreds of kilometers deep. Such a cavity is not stable because differential stresses in the surrounding rocks reach $10^9$ Pa or more. Melosh and McKinnon speculated that the inward flow of the underlying mantle may be responsible for the mountainous rings surrounding large lunar basins, a speculation that is now supported by the model by Johnson et al. of the formation and collapse of the Moon’s Orientale basin, a computation that used the algorithm described in this paper.

1.1 THE iSALE HYDROCODE

The hydrocode iSALE is a multi-material shock physics code (historically called a “hydrocode,” although iSALE and most modern codes incorporate more than hydrodynamic flow). It solves the Navier-Stokes equations in a compressible fashion on a Cartesian staggered mesh grid by using finite differences and finite volumes in either two or three dimensions. The solver follows the scheme of Hirt et al., which allows the calculation of flows at nearly arbitrary speeds. The simulations can be performed in a Eulerian or Lagrangian fashion as well as by using an Arbitrary Lagrangian Eulerian (ALE) technique. For calculations of meteorite impacts, however, the large strains would greatly distort a Lagrangian mesh, making the Eulerian approach the most reasonable one. As in most such codes, time is advanced via an explicit algorithm, so that cell variables at a given time $t$ are advanced to the next time step at $t + \Delta t$ using the current values of pressure, stress, and velocity to compute accelerations and, hence, new velocities and positions at the next step, until a final specified time is reached. The code employs a number of different equations of state, such as the Analytical Equation of State (ANEOS) or Tillotson, allowing computations with a realistic thermodynamic behavior for many geomaterials. In addition, different constitutive models are required to account for material strength, damage and failure, porosity, dilatancy, acoustic fluidization, thermal softening, or low-density weakening.

The underlying constitutive model, however, is either elasto-plastic or purely viscous (simple linear and time-independent viscosity). A visco-elastic or even visco-elasto-plastic rheology has not been considered previously. The development and implementation of this extension is presented in the subsequent sections.
2 | Viscous Flow Mechanisms—Descriptions

The rheology of rocks depends on a large number of constitutive and environmental factors, including mineralogy, fluid content and chemistry, mineral grain size, melt fraction, temperature pressure, and differential stress conditions. The same is true for the viscous behavior of, for example, the Earth’s interior: while the upper crust is usually assumed to be in a frictional equilibrium with active faults that might limit the strength, the pressure-dependent increase of frictional strength with increasing temperature and depth, work in opposite directions.

A simple linear viscous rheology is not sufficient for a realistic calculation of mantle behavior. We therefore use a more sophisticated model that has been previously presented in several papers. This model consists of three different regimes depending on stress and temperature: grain-size dependent diffusion creep; a power-law dislocation creep; and the exponential Peierls mechanism for larger stresses and strain rates, such as during meteorite impact and the subsequent collapse of the initial deep crater.

In our approach, the overall strain rate, $\dot{\varepsilon}_v$, due to inelastic deformation consists of a sum of viscous strain rates due to the three creep mechanisms, that is, diffusion creep ($\dot{\varepsilon}_1$), dislocation (or power-law) creep ($\dot{\varepsilon}_n$), and Peierls creep ($\dot{\varepsilon}_p$):

$$\dot{\varepsilon}_v = \dot{\varepsilon}_1 + \dot{\varepsilon}_n + \dot{\varepsilon}_p.$$  \hfill (1)

Note that, here and in the following section, we express strain and stress in a generalized fashion, suppressing tensor indices for clarity. The full tensor expressions will be displayed in several of the equations noted below. Also recall that these expressions refer only to the deviatoric stresses and strains, that is, the portions of the stress and strain tensors that exclude the volume strain and pressure. These variables are generally handled separately in hydrocodes, where the volume strain (inverse density) and pressure are linked through a thermodynamic equation of state. The rheologic behavior of material is treated separately as part of the constitutive model that describes the materials’ response to the differential stresses which correspond to a change of shape, rather than to a change of volume.

Diffusion creep accounts for deformation of material by diffusion of vacancies in the crystal lattice. It is therefore a plastic deformation, which gives rise to ductile, not brittle, behavior. It is generally a linear function of stress. The strain rate due to diffusion creep depends not only on temperature $T$ and deviatoric stress $\sigma$ (this is usually taken equal to the square root of the second invariant of the stress tensor, as the appropriate generalization of shear stress), but also on grain size $a$:

$$\dot{\varepsilon}_1 = \frac{\sigma}{\eta_0} \left( \frac{a}{a_0} \right)^{-m} \cdot \exp \left( -\frac{E_1}{R \cdot T} \right),$$  \hfill (2)

where $a_0$ is the reference grain size (here: $a_0 = 1$ mm), $R$ is the gas constant, $\eta_0$ is a reference viscosity, and $E_1$ is an activation enthalpy. $m$ is a material-dependent parameter describing the grain size-dependency of diffusion creep, which ranges between 2, for volume diffusion (Nabarro-Herring creep), and 3, for grain boundary diffusion (Coble creep). Diffusion creep is mainly important at lower stresses, is highly temperature-dependent, and results in very small strain rates.

Dislocation creep (power-law creep) describes material deformation as the result of dislocations moving through the crystal lattice. It is best described by a power-law function of the deviatoric stress, in which the strain rate depends on temperature and stress but is independent of the grain size:

$$\dot{\varepsilon}_n = \frac{\sigma_c}{\eta_0} \left( \frac{\sigma}{\sigma_c} \right)^n \cdot \exp \left( -\frac{E_n}{R \cdot T} \right).$$  \hfill (3)

Here $E_n$ is the activation enthalpy of non-Newtonian creep, $\sigma_c$ is the critical stress for dislocation motion, and $n$ is the exponent for the power-law dependence of this creep, that usually ranges between 3 and 5. This mechanism usually predominates at intermediate stresses and higher temperatures.

The Peierls mechanism is a special type of dislocation creep that is thermally activated and dominates only at high deviatoric stress. This mechanism depends on the thermally activated unpinning of dislocations that are pushed far out of their minimum-energy configurations by high applied stresses. While thermally activated, this mechanism depends less upon temperature and more upon stress than dislocation creep. The creep law for the Peierls mechanism is given by:

$$\dot{\varepsilon}_p = A_p \cdot \exp \left[ -\frac{E_p}{R \cdot T} \left( 1 - \frac{\sigma}{\sigma_p} \right)^q \right].$$  \hfill (4)
where $A_P$ and $q$ are material-dependent parameters, $E_P$ is the activation enthalpy for the Peierls mechanism, and $\sigma_P$ is the Peierls stress. Peierls creep dominates for stresses above 500 MPa, although this depends upon the material. Mantle materials such as olivine are much more susceptible to Peierls creep than typical crustal minerals such as plagioclase, which is why this mechanism may play a particularly important role in the collapse of impact basins on the terrestrial planets.

The parameters in the equations shown above are strongly material dependent. Because our study focuses on mantle rheology we chose values that best reflect dry olivine, as in the 1999 work by Kameyama et al. See Table 1 below for the parameter values.

Expanding Equations (1) to (4), the overall viscous strain rate is given by

$$
\dot{\varepsilon}_\nu = \frac{\sigma}{\eta_0} \left( \frac{a}{a_0} \right)^{-m} \exp \left( -\frac{E_1}{RT} \right) + \frac{\sigma_c}{\eta_0} \left( \frac{\sigma}{\sigma_c} \right)^n \exp \left( -\frac{E_n}{RT} \right) + A_P \cdot \exp \left[ -\frac{E_P}{RT} \left( 1 - \frac{\sigma}{\sigma_P} \right)^q \right].
$$

(5)

The deformation map in Figure 1 shows the relationship between strain rate, stress, and temperature as given by Equation (5). We can clearly see that the diffusion creep only accounts for strain rates which are (usually) much smaller than those expected for large-scale planetary impact events, except for much slower viscous relaxation long after the crater forms. Thus, it is likely that diffusion creep does not play an important role for this study, where typical strain rates in large impacts range from $1 \times 10^{-3}$ to 10 seconds$^{-1}$. For performance reasons, Equation (2) might be neglected if applied according to Equation (5). The parameter space dominated by each of the terms in Equation (5) is denoted by different hues, depending on strain rate. Note that the original equations implicitly include a pressure dependence in the enthalpy term, which is not strong and therefore neglected here. The diffusion regime (blue) is highly temperature dependent and important for small strain rates only. Dislocation creep (beige) occurs for intermediate stresses and higher temperatures, while the Peierls mechanism (green) dominates at higher stresses (>500 MPa) and shows a strong stress dependence for low temperatures. The labeled contours are Log10 strain rate in units of seconds$^{-1}$.
for planetary scale impact simulations. In the framework of this study, however, we included this mechanism for completeness. Instead we ignored a possible pressure dependence in the Peierls regime (as, for example, suggested by Kawazoe et al\textsuperscript{54}), because it is much smaller than the temperature and stress dependence for the simulations intended within the framework of our study. Indeed, if long-term crater relaxation is the goal of a simulation, then iSALE is a poor choice, because the inclusion of inertial accelerations in iSALE requires very small time steps that would be impractical for deformation occurring over millions of years. When such a problem arises, the best option is to use a pair of codes sequentially, such as iSALE followed by a finite element analysis that utilizes long-term creep rheology, like in the work by Freed et al.\textsuperscript{59}

3 COUPLING VISCOUS FLOW WITH AN ELASTO-PLASTIC MODEL

The time dependence of the response of a viscoelastic system is similar to that of an electrical circuit. From a mathematical perspective both systems can be described by an identical set of ordinary differential equations. A convenient approach to this problem is the so-called “spring-dashpot” model, where the elastic rheology is represented by an elastic spring, described by

$$\sigma = 2\mu \cdot \varepsilon. \quad (6)$$

where $\sigma$ and $\varepsilon$ represent the spring force and strain, respectively, and $\mu$ is the shear modulus. The factor 2 in this and latter equations is a conventional link between the engineering definition of shear strain and the tensor definition that we employ here.

The viscous rheology can be visualized by a Newtonian dashpot:

$$\sigma = 2\eta \cdot \dot{\varepsilon}. \quad (7)$$

where $\eta$ is the viscosity. These two basic elements can be combined in different ways to simulate more complex rheologic behavior.

Following this approach, different rheologic models are generally used. The Maxwell-configuration connects one spring and one dashpot in series, so that the strain is the sum of each element while the stress is the same in both. The Kelvin-Voigt puts a viscous and an elastic element in parallel so that the strain is equal in both elements while the total stress is the sum of the individual stresses. A Standard Linear Solid combines a Maxwell element and a spring in parallel. To describe a more complex rheology such as that of polymers, mathematical solutions have been presented that rely upon arbitrary combinations of multiple elements.\textsuperscript{60-62}

We used a Maxwell-configuration in conjunction with a plastic flow model to connect the viscous creep rheology as described above to an elasto-plastic model to allow visco-elastic or even visco-elasto-plastic material behavior. This configuration is shown schematically in Figure 2.

When using elasticity, viscosity, and plasticity in series, every element in the entire system experiences the same stress, while the strain rates are additive:

$$\sigma_T = \sigma_V = \sigma_E = \sigma_P, \quad (8)$$

$$\dot{\varepsilon}_T = \dot{\varepsilon}_V + \dot{\varepsilon}_E + \dot{\varepsilon}_P. \quad (9)$$

Here, the subscripts $T$, $V$, $E$, and $P$ refer to the total, viscous, elastic, and plastic contributions, respectively. The constitutive equation for viscoelasticity in a Maxwell-configuration is directly inherited from Equations (6), (7), and (9):

$$\dot{\varepsilon} = \frac{1}{\mu} \sigma + \frac{1}{\eta} \dot{\sigma}. \quad (10)$$

**FIGURE 2** Schematic illustration of the Maxwell elasto-visco-plastic rheology solved by our algorithm. The total strain (between the dots at the extreme ends of the chain) is defined as the sum of the strains in each of the elastic, viscous, and plastic elements. The stress acts equally in each of the elements. In our model the viscous element includes both linear viscous (Newtonian) rheology, power law dislocation creep and exponential Peierls-mechanism creep.
The advantage of utilizing a Maxwell-model is that it permits relaxation of stresses, while allowing arbitrarily large
 strains, consistent with the behavior of geologic materials. For example, under the condition of strain that is suddenly
 applied and then held fixed, the stress relaxes by

$$\sigma(t) = \sigma_0 \cdot e^{-t/T_M},$$ (11)

where $T_M = \frac{n}{\mu}$ is the Maxwell decay time.\textsuperscript{15}

4 | IMPLEMENTATION OF VISCO-ELASTO-PLASTICITY IN A HYDROCODE

The constitutive equation for viscous creep, Equation (5), shows how to calculate the strain rate from a given stress.
However, the hydrocode we utilize for our study, iSALE, works in the opposite way: it updates the stresses from a given
strain rate. This creates two complications that must be solved:

1. The constitutive Equation (5) must be inverted to compute the stress from a given strain rate. Because this is a
transcendental equation, it must be solved numerically, which is very time-consuming.
2. Because we calculate the stress contributions from the total strain rates and we assume that each element acts in
series, we need to determine the correct partitioning of the total strain rate ($\dot{\varepsilon}_T$) into an elastic strain rate ($\dot{\varepsilon}_e$), a viscous
strain rate ($\dot{\varepsilon}_\nu$), and a plastic strain rate ($\dot{\varepsilon}_p$).

   In the series configuration the same stress acts on each element, which responds with its own strain rate, according
to the size of each term in Equation (5). Please note that, when we use the deviatoric stress and strain, these equations
hold separately for each component of the stress and strain.

In the following, we present an approach to deal with these issues. This approach to the computation of
visco-elasto-plastic behavior requires five different steps which are described in this section:

1. Derive an effective viscosity from the previous stress.
2. Calculate an effective stress from the effective viscosity.
3. Use the effective stress to calculate the corresponding viscous and elastic strain rates.
4. Reduce the stress and update strain rates if the stress exceeds the yield envelope (plastic deformation).
5. Compute the elastic strain (as opposed to strain rate) from the final deviatoric stress and the elastic constitutive
   equation.

These steps and their application in the hydrocode are outlined in Figure 3, where the level of each step is explicitly
shown. The actual equations for the algorithm outlined in Figure 3 are detailed in the sections below.

4.1 | DERIVE AN EFFECTIVE VISCOSITY

For viscous material behavior, we consider diffusion creep, dislocation creep, and Peierls creep. The strain rate due to
each mechanism is additive, which results in the main Equation (5). Note that most experimenters use pure shear, so they
measure $2 \cdot \dot{\varepsilon}_{ij}$ and not $\dot{\varepsilon}_{ij}$. Thus, our basic equation is

$$2 \cdot \dot{\varepsilon}_\nu = \left( \frac{a}{a_0} \right)^{-m} \frac{\sigma}{\eta_0} e^{-\frac{\sigma}{k_B T}} + \frac{\sigma_c}{\eta_0} \left( \frac{\sigma}{\sigma_c} \right)^n e^{-\frac{\sigma}{k_B T}} + A_P \cdot e^{-\frac{\sigma}{k_B T} \left( 1 - \frac{\sigma}{\sigma_P} \right)^2}. \quad (12)$$

Explicitly displaying the full tensor indices for the deviatoric strains and stresses, we rewrite this equation as below:

$$2\dot{\varepsilon}_{ij} = \left[ \frac{1}{\eta_0} \left( \frac{a}{a_0} \right)^{-m} e^{-\frac{\sigma}{k_B T}} + \frac{1}{\eta_0} \left( \frac{\sigma_c}{\sigma_c} \right)^n e^{-\frac{\sigma}{k_B T}} + A_P \cdot e^{-\frac{\sigma}{k_B T} \left( 1 - \frac{\sigma}{\sigma_P} \right)^2} \right] \sigma_{ij}. \quad (13)$$
**FIGURE 3** Flowchart illustrating the implementation of our elastic-visco-plastic algorithm during the execution of hydrocode. At the beginning of each cycle the hydrocode provides the current pressure and velocities, computed from the set of Navier-Stokes equations. The total strain rate is computed from the velocity field and the deviatoric stresses are known from the previous cycle at the initial time $t_0$. These variables are advanced by the time step $\Delta t$ during the course of this computation, and the new deviatoric stresses are incorporated into the Navier-Stokes equations for the next time step.

Here, the invariant shear stress $\sigma_2$ is the square root of the second invariant of the stress tensor. Considering the constitutive equation for the viscous element

$$\dot{\varepsilon}_{ij} = \frac{1}{2\eta} \sigma_{ij},$$

we can easily compute an effective viscosity $\eta_{\text{eff}}$ at any working stress $\sigma$:

$$\frac{1}{\eta_{\text{eff}}} = \frac{1}{\eta_0} \left( a \frac{a_0}{A_0} \right)^m e^{-\frac{\varepsilon_0}{\bar{T}}} + \frac{1}{\eta_0} \left( \frac{\sigma_2}{\sigma_e} \right)^{n-1} e^{-\frac{\varepsilon_0}{\bar{T}}} + \frac{A_P}{\sigma_2} e^{-\frac{\varepsilon_0}{\bar{T}}} \left( 1 - \frac{\sigma_2}{\sigma_e} \right)^2.$$  \hspace{1cm} (15)

Here, we use the stress tensor $\sigma_i(t_0)$ at the beginning of the current cycle as a reference stress.

### 4.2 | CALCULATE THE EFFECTIVE STRESS

At the beginning of each time step we know the previous stress $\sigma_i(t_0)$. In our approach, the viscosity only contributes to the stress of material whose stress does not exceed the yield envelope, $Y$ (ie, $\sigma_2 < Y$). Because the stress in the previous step was, at worst, just on the yield curve, we assume, for the moment, that the plastic strain is zero ($\dot{\varepsilon}_p = 0$). This assumption will be revisited at the end of the current cycle and any necessary corrections applied. For the current (ie, new) time step, we therefore know

$$\dot{\varepsilon}_T = \dot{\varepsilon}_v + \dot{\varepsilon}_e \quad (\dot{\varepsilon}_p = 0).$$

Using the constitutive Equations (6) and (7), we obtain

$$\dot{\varepsilon}_T = \frac{1}{2\mu} \sigma + \frac{1}{2\eta} \sigma.$$  \hspace{1cm} (17)
Please note that here we use the effective viscosity \( \eta = \eta_{\text{eff}} \). The differential equation for \( \sigma \) is given by

\[
2\mu \dot{\varepsilon} = \frac{d\sigma}{dt} + \frac{\mu}{\eta} \sigma = \frac{d\sigma}{dt} + \frac{\sigma}{T_M}.
\]  

(18)

being \( T_M \) the Maxwell decay time defined above. This equation possesses a general solution given by

\[
\sigma(t) = \sigma(t_0) e^{\frac{e^{\frac{\eta}{2\mu} t}}{T_M}} + e^{\frac{\mu}{T_M} \int_{t_0}^{t} \dot{\varepsilon}_T(t') \cdot 2 \mu \cdot e^{\frac{\eta}{2\mu} t'} dt'}.
\]  

(19)

If \( t - t_0 = \Delta t \) is short, and we assume that \( \dot{\varepsilon}_T(t) \) is constant over \( t_0 \) to \( t_0 + \Delta t \), then

\[
\sigma(t) = \sigma(t_0) e^{\frac{\eta}{2\mu} \Delta t} + 2\mu \dot{\varepsilon}_T(t_0) \left( 1 - e^{\frac{\eta}{2\mu} \Delta t} \right) - \frac{\Delta t}{T_M}.
\]  

(20)

\[
\sigma(t) \approx \sigma(t_0) \left( 1 - \frac{\Delta t}{T_M} \right) + 2\mu \dot{\varepsilon}_T \Delta t,
\]  

(21)

\[
\sigma(t) \approx \sigma(t_0) \left( 1 - \Delta t \right) + 2\mu \dot{\varepsilon}_T \Delta t,
\]  

(22)

to first order in \( \Delta t \). Now we can use Equation (22) to calculate the effective stress from the effective viscosity, which determines \( T_M \).

### 4.3 PARTITIONING VISCOUS AND ELASTIC STRAIN RATES

By using the derived effective stress, we can now compute the elastic and viscous strain rates. From the definition of elastic strain (Equation (6)) and Equation (22) for the stress change in this cycle, the elastic strain rate is given by

\[
\dot{\varepsilon}_e = \frac{1}{2\mu} \sigma = \frac{1}{2\mu} \left( -\sigma(t_0) \frac{\Delta t}{T_M} + 2\mu \Delta t \dot{\varepsilon}_T \right) \cdot \frac{1}{\Delta t}.
\]  

(23)

Simplifying and using the definition of \( T_M \), one yields:

\[
\dot{\varepsilon}_e = -\frac{1}{2\eta} \sigma(t_0) + \dot{\varepsilon}_T ,
\]  

(24)

which, using Equations (15) and (22), yields the strain rate in the viscous element:

\[
\dot{\varepsilon}_v = \frac{1}{2\eta_{\text{eff}}} \sigma(t) = \frac{1}{2\eta_{\text{eff}}} \sigma(t_0) \left( 1 - \frac{\Delta t}{T_M} \right) + \frac{\dot{\varepsilon}_T}{T_M} \Delta t.
\]  

(25)

### 4.4 PLASTICITY—RHEOLOGY ON THE YIELD ENVELOPE

Finally, we compare the new stress (here: the square root of the second invariant \( \sigma_2 \)) with the yield envelope. If \( \sigma_2 < Y \), no plastic strain occurs, and the total strain rate is partitioned into elastic and viscous strain rates as given in Equation (23), (24). If the stress exceeds the yield limit (ie, \( \sigma_2 \geq Y \)), then stresses are relaxed to the yield envelope

\[
\sigma_{ij}^{\text{new}} = \frac{Y}{\sigma_2} \sigma_{ij}(t),
\]  

(26)
and, once the new stress is known, we again use the constitutive equations (Equations (6) and (7)) to compute the new (reduced) elastic $\dot{\varepsilon}_e$ and viscous $\dot{\varepsilon}_\nu$ strain rates at the new stress on the yield envelope:

$$\dot{\varepsilon}_e = \frac{1}{2\mu} \dot{\sigma}_ij^{\text{new}},$$

$$\dot{\varepsilon}_\nu = \frac{1}{2\eta} \dot{\sigma}_ij^{\text{new}}.$$  

(27)

(28)

The remaining part contributes to the current plastic strain rate (see Equation (9)):

$$\dot{\varepsilon}_p = \dot{\varepsilon}_T - \dot{\varepsilon}_e - \dot{\varepsilon}_\nu.$$  

(29)

At the end of each cycle, the total strains due to the viscous and plastic flow are incremented by the strain rates multiplied by the time step and stored. The plastic strain as a function of time is particularly useful for tracking the material flow.

5 RESULTS AND VERIFICATION

To test and explore our rheology model, we performed numerical simulations of a 1-m sized block sheared with a velocity of 1 m/s and recorded the resulting stresses and effective viscosities. While this test becomes quite unrealistic after strains exceed a few tens of percent, it provides a stringent test of the stability of our numerical method. The block is composed of dunite. To calculate its thermodynamic behavior, we used the ANEOS equation of state with tabularized data for dunite. For the viscous calculations, we used the same parameters as those listed in Table 1. We assumed a preheated block at an initial temperature of 1700 K and pressure of 0.30 GPa to focus on the regime where the Peierls creep becomes important (see Figure 1). This temperature also better reflects the thermal conditions in the Earth’s mantle.

The total elastic strain contribution at this time $\varepsilon_e(t)$ is calculated at this time from the final stress from its definition (Equation (6)):

$$\varepsilon_e = \frac{1}{2\mu} \sigma_{ij}^{\text{new}},$$

where the elastic shear modulus $\mu$ is computed from the speed of shear waves and density, and thus depends on the thermodynamic behavior of the material. At the conditions described above, it is on the order of 130 GPa.

The plastic behavior is simulated by limiting stresses to the yield envelope and reducing strain rates properly (see Section 4.4). The iSALE hydrocode contains different methods for calculating the yield envelope of a given material. For these tests, we utilized the so-called rock-model. In this model, the yield envelope comprises different stress paths for intact and damage material. While the yield envelope for completely damaged material is calculated by using a simple Mohr-Coulomb approach, intact material is represented by a Lundborg relationship. Between these two states a linear interpolation is used to retrieve an adequate yield limit. The parameters used for this plasticity model are listed in Table 2.

We calculated the shearing of the block for different material rheologies: (i) purely elastic; (ii) elasto-plastic; (iii) visco-elastic; and (iv) visco-elasto-plastic, assuming an overall pressure of $3 \times 10^8$ Pa. The results are shown in Figures 4-8. Stresses and strain rates are always represented by their XY-component. Figure 4 shows the time evolution of stress for all four different rheologies. While a purely elastic rheology results in a significant and continuous stress increase, stresses in the elasto-plastic regime are significantly lower. In the latter case, the resulting stresses always lie on the yield envelope, which through the strength model of Collins et al is temperature-dependent and so the stress declines as plastic work heats the material. Thus, when considering elasto-plastic behavior, plastic work, and plastic strain occur at all times during deformation.

A comparison between the elastic and visco-elastic behavior reveals an identical stress evolution in the very early stage. Later on, however, stresses begin to relax in the viscoelastic case. The rate of the stress decay is defined by the Maxwell time $T_M = \eta_{\text{eff}}/\mu$ which describes the time required to decrease the stress to $1/e$ of the initial stress. In laboratory experiments, this measure is often used to obtain insights into the viscous behavior of a given material. In our approach, however, the Maxwell time is itself time-dependent because the effective viscosity $\eta_{\text{eff}}$ varies with time due to its dependence on stress and temperature, as shown in Figure 5. In this experiment, the Maxwell time quickly declines from 35 seconds in the
| Parameter                                      | Value                                      |
|------------------------------------------------|--------------------------------------------|
| Poisson ratio                                  | 0.3                                        |
| Equation of state                              | ANEOS for dunite                           |
| Specific heat capacity                         | 1000 (J kg\(^{-1}\) K\(^{-1}\))           |
| Shear strength at initial condition (intact material) | 10\(^7\) (Pa)                              |
| Coefficient of internal friction (intact material) | 1.1                                        |
| Shear limit (Intact material)                  | 2.5 \(\times\) 10\(^9\) (Pa)              |
| Shear strength at initial condition (damaged material) | 10\(^4\) (Pa)                              |
| Coefficient of internal friction (damaged material) | 0.8                                        |
| Shear limit (damaged material)                 | 2.0 \(\times\) 10\(^9\) (Pa)              |

**TABLE 2** Parameters used to describe the elasto-plastic and thermal behavior of dunite

**FIGURE 4** Evolution of stress during shearing for elastic (blue dashed line), elasto-plastic (red dashed line), visco-elastic (blue solid line), and visco-elasto-plastic (red solid line) material behavior. The black arrow on the left axis indicates the plastic yield stress at the ambient pressure of 0.3 GPa for a fully damaged material. The rollover of the elastic stresses after about 0.1 seconds is due to the extreme distortion of the initial 1 \(\times\) 1 \(\times\) 1 m cube of dunite (the strain is 10% at 0.1 second). At 1 second, the total strain is 100% and continues to increase thereafter as the block is distorted from a cube into a long parallelepiped. Our algorithm nevertheless faithfully follows the stress evolution in this distorted block. Note that in our rheological model the stress is the same in each element of the system, so the stress plotted acts equally on the elastic, viscous, and plastic elements.

**FIGURE 5** Effective viscosity and corresponding Maxwell time for viscoelastic material behavior during shearing (\(T=1700\) K). The elapsed time \(t\) is plotted as a dashed line (referred to the right-hand axis) to illustrate whether the current time exceeds the corresponding Maxwell time or not. The two are equal at about 0.047 second.
**FIGURE 6** Viscous and elastic stress increments during shearing for the viscoelastic example in Figure 4 (T = 1700 K). Note that the magnitude of the contributions depends on the time increment $\Delta t$, as in Equations (31)-(33).

**FIGURE 7** Temperature dependence of elastic and viscoelastic material rheology. The right panel shows an expanded section of the initial stage.

**FIGURE 8** Dependence of the evolution of effective viscosity during shearing on temperature.
beginning to less than 30 ms after 0.1 second from the beginning of the shearing process. At the same time, the effective viscosity decreases over three orders of magnitude from \( > 10^{12} \) Pa-s to \( 10^9 \) Pa-s.

Our Maxwell-type rheology model (Figure 2) is constructed on the assumption that the stresses in each of the three major elements (ie, elastic, viscous, and plastic) are equal at all times. However, the structure of Equation (22) for the stress change during the current cycle contains two terms, one of which could be construed as an elastic contribution to the stress and the other to a viscous contribution. This is supported by mathematical models in which the total strain is applied to the elastic element instantaneously at the beginning of the time step, after which the viscous element is permitted to relax the stress at a rate governed by the Maxwell time \( T_M \). We can thus identify two terms in the stress change which we will call the elastic increment \( \Delta \sigma_e \) and the viscous increment \( \Delta \sigma_v \). Please note, however, that the same stress acts in both elements at all times: this is a mathematical separation, albeit useful for understanding the relative contributions of either elastic or viscous processes. In these terms, the new stress at the end of a time step is given by:

\[
\sigma(t_0 + \Delta t) = \sigma(t_0) + \Delta \sigma_e - \Delta \sigma_v,
\]

where the individual terms, derived from Equation (22), are given by:

\[
\Delta \sigma_e = 2\mu \dot{\varepsilon} T \Delta t,
\]

\[
\Delta \sigma_v = \sigma(t_0) \frac{\Delta t}{T_M} = \sigma(t_0) \frac{\mu \Delta t}{\eta_{\text{eff}}}.
\]

Figure 6 shows these individual contributions to the stress during the course of our example computation. Note that the magnitude of these contributions depends linearly on the size of the time increment (\( \Delta t \), as Equations (32) and (33) require. Also note the negative sign in the viscous term of Equation (31) indicates that the viscous contribution lessens the instantaneous elastic stresses. As is also evident in Figure 6, the rheology is initially dominated by elastic (or elasto-plastic) behavior. The viscous relaxation is significantly lower than the elastic stress but increases rapidly. Thus, very shortly after the onset of shearing, viscous relaxation becomes more prominent than the elastic contributions. The stress therefore decays. This happens roughly when the Maxwell time and the current time step are the same (at the intersection between the Maxwell decay time and the decay limit in Figure 5). The dominance of the viscous contributions results in a quick decay of the total stresses. While the elastic stresses increase slowly, the viscous stresses decrease after reaching their maximum. Thus, the decrease of stress is also damped by time, in agreement with Equation (11).

When considering a full visco-elasto-plastic rheology, the material initially behaves as purely elasto-plastic (see Figures 2 and 4) because there is not enough time for viscous strains to accumulate. The resulting stresses in the visco-elasto-plastic scenarios are exactly the same until the block is strongly deformed and the yield stress is exceeded. Despite stress relaxation in the viscous element (and the corresponding accumulation of viscous strain), the resulting stresses remain on the yield envelope during large parts of the deformation. Stresses are, thus, reduced (see Section 4.4) and part of both the viscous and elastic strain is converted into plastic strain. At some time later, however, the viscous flow relaxes the stress below the yield envelope. From this moment on, the resulting stress veers away from the yield envelope and the material behaves as purely visco-elastic.

All three regimes considered by us to calculate a realistic viscous behavior (ie, diffusion creep, dislocation creep, and the Peierls mechanism) depend on temperature, as well as stress. Each of these regimes is activated or dominant at different temperature conditions, as Figure 1 illustrates. Thus, we repeated the experiments described above and systematically varied the initial temperature of the block material.

Figure 7 shows the stress evolution for both purely elastic (dashed lines) and visco-elastic (solid lines) material behavior and for different temperatures. It is evident that the resulting stresses decrease with increasing temperatures. If only the viscous behavior is considered, however, the stresses are much lower and even the temperature dependence on stress is much more pronounced. Furthermore, the separation of the visco-elastic path from the purely elastic path occurs much earlier for higher temperatures, as visible in Figure 7 (right), which shows the stress evolution for the very early stages. This observation is also demonstrated in Figure 8 showing the effective viscosity as a function of time. The initial viscosity is much higher for lower temperatures. At room temperature, the resulting initial viscosity \( \eta_{\text{eq}}(t \approx 0) \) is above \( 10^{60} \) Pa-s and the material behaves therefore more solid-like until the viscosity starts to decrease after some time due to the stress dependence of the viscosity. The onset of a significant and nonlinear decrease of the viscosity depends strongly on temperature and occurs much earlier for higher temperatures. At a temperature of 2000 K, the initial viscosity drops to \( 10^{10} \) Pa-s.
and the viscous effects are therefore more prominent right from the beginning of the deformation. Despite the different temperature conditions, all viscosities asymptotically approach the same value at a later stage (i.e., \( \approx 10^{10} \) Pa·s). The resulting stresses for \( T = 2000 \) K are slightly slower, which can be explained by the onset of changes in the thermodynamic behavior (beginning phase transitions) at conditions close to the melting point of dunite.

6 | SUMMARY AND DISCUSSION

We have presented a simple and efficient way of implementing a viscous creep rheology based on diffusion creep, dislocation creep, and the Peierls mechanism in conjunction with an elasto-plastic rheology model into a shock-physics code. The three regimes are combined continuously, that is, there is no threshold initiating a sudden change from one regime to the next. While the viscoelasticity of the mantle as utilized for mantle convection or other slow geodynamic or geological processes is mostly controlled by diffusion and dislocation creep, the Peierls mechanism becomes the dominant mechanism at the large stresses and strain rates occurring during meteorite impacts and other highly dynamic processes where differential stresses become very high.

Our approach to implementing the model into the shock-physics-code iSALE is based on the calculation of an “effective viscosity” which is then used as a reference viscosity for any underlying viscoelastic (or even visco-elasto-plastic) model. Here, we use a Maxwell-configuration, where elastic, viscous, and plastic strain rates sum up to the total strain rate and the stress contributions at the viscous, elastic, and plastic elements are identical. The Maxwell-model best describes stress relaxation (see Equation (11)) in natural materials, and hence is likely to be important for the formation of large meteorite impact basins, for which this code was intended. However, this model does not consider the full range of observed creep phenomena accurately. Under constant stress conditions, strain in this model increases linearly with time. Most natural materials, however, exhibit a more complex relationship and at lower temperatures strain rates usually decrease with time, in a regime known as primary creep. The Kelvin-Voigt approach, where the viscous and elastic elements are arranged in parallel (and, thus, each element encounters the same strain rate, but the resulting stresses sum up to the total stress), simulates creep at small strains much more accurately, but it is less accurate for predicting large strain behavior. In the last decades, more complex rheologies have been developed and proposed, such as the Standard-Linear-Solid (where a Maxwell-model is combined with an additional elastic element in parallel) or a Generalized Maxwell Model or Maxwell-Wiechert model (arbitrary number of Maxwell-elements in parallel\(^{60-62}\)). Our approach of calculating an effective viscosity can easily be applied to more complex configurations, which we intend to do in future work.

In the meantime, the algorithm described in this paper has been incorporated into the developer version of iSALE and is used in the form described here by Johnson et al.\(^{62}\) and Lyons et al.\(^{64}\) A version modified for ice rheology appeared in Johnson et al.\(^{65}\), Silber et al.\(^{66}\) and Bowling et al.\(^{67}\) We anticipate that future publications will use this rheology as the developer version of iSALE is migrated to the user version.

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AUTHOR CONTRIBUTIONS

Dirk Elbeshausen: Formal analysis; methodology; software; validation; writing-original draft. Henry Melosh: Conceptualization; project administration; supervision; writing-review and editing.

CONFLICT OF INTEREST

The authors declare no potential conflict of interest in this work.
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