Dynamic behavior of nano-voi ds in magnesium under hydrostatic tensile stress

Mauricio Ponga1, Amuthan A Ramabathiran2, Kaushik Bhattacharya2 and Michael Ortiz2

1 Department of Mechanical Engineering, University of British Columbia, 2054—6250 Applied Science Lane, Vancouver, BC, V6T 1Z4, Canada
2 Division of Engineering and Applied Science, California Institute of Technology, 1200 E. California Blvd., Pasadena, CA, 91125, USA

E-mail: mponga@mech.ubc.ca, amuthan@caltech.edu, bhatta@caltech.edu and ortiz@aero.caltech.edu

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Abstract
We investigate the mechanisms responsible for nano-void growth in single crystal magnesium under dynamic hydrostatic tensile stress. A key conclusion derived from our study is that there is no secondary strain hardening near the nano-void. This behavior, which is in remarkable contrast to face-centered cubic and body-centered cubic materials, greatly limits the peak stress and explains the relatively lower spall strength of magnesium. The lack of secondary strain hardening is due to the fact that pyramidal dislocations do not interact with basal or prismatic dislocations. Our analysis also shows that for loads applied at moderate strain rates ($\dot{\varepsilon} \leq 10^6 \text{s}^{-1}$) the peak stress, dislocation velocity and temperature distribution converge asymptotically. However at very high strain rates ($\dot{\varepsilon} \geq 10^8 \text{s}^{-1}$), there is a sharp transition in these quantities.

Keywords: material failure, ductility, plasticity, thermal conductivity, dislocations in magnesium

(Some figures may appear in colour only in the online journal)

1. Introduction

As the lightest of all metallic materials and one of the most abundant elements in the earth’s crust, magnesium (Mg) and its alloys offer tremendous potential for lightweight structural engineering to satisfy the strong demand of weight reduction of transportation vehicles,
human prostheses, electronic devices, etc. At present, however, the limited range of mechanical properties like poor formability and low yield strength of the various types of magnesium alloys available hinders widespread industrial use of these materials [1–3].

This is largely a consequence of the hexagonal close-packed (HCP) lattice structure of Mg. The HCP structure has four independent slip systems, viz. two basal \( \{0001\} \) and two prismatic \( \{10\bar{1}0\} \) slip systems. It also has pyramidal slip systems with components in \( \langle a \rangle \) and \( \langle c \rangle \)-directions; these can be obtained as a linear combination of the aforementioned slip systems [4, 5]. A key issue in HCP metals is that the critical stress for dislocation activity in the prismatic and pyramidal systems is at least one order of magnitude higher than that in the basal system [6–8]. Though dislocation activity can be supplemented by twinning to accommodate deformation along the \( \langle c \rangle \)-direction [9], this extreme contrast between basal and other deformation modes leads to a high anisotropy, low yield strength, high shear localization and poor formability in comparison with other metallic materials.

In this work we study the deformation mechanisms operative in Mg during dynamic failure since various proposed applications involve high strain rates. Our goal is to shed light on the mechanisms that dominate this mode of failure and thereby provide insights that can be used to inform the design of new Mg-based alloys.

Dynamic failure is a complex phenomenon that occurs when a material is subject to high strain rates and is characterized by a strongly coupled thermo-mechanical evolution of a macroscopic crack through the nucleation, growth and coalescence of nano- and micro-voids. Under these conditions, the material usually fails by spallation [10–12]. Spallation occurs when two release waves collide in the aftermath of a compressive shock load. The collision of two release waves produces a tensile stress that increases rapidly in a very narrow plane inside the material, usually called the spall plane. The tensile stress acts on vacancies and clusters of vacancies promoting nucleation, growth and coalescence of nano-voids that, eventually results in a macroscopic crack in the matrix, thereby compromising the structural integrity of the specimen [12–15]. One of the major difficulties that appears in the experimental characterization of spallation is that most of the experimental observations are restricted to free-surface velocity measurements and post mortem examination of the specimens, and therefore are necessarily indirect [16, 17]. In addition, the experimental characterization of spallation in Mg, and HCP materials in general, yet remains largely open with only a few experimental data available in the literature (see [18] and references therein).

2. Methodology

2.1. HotQC method

Numerical simulations provide a highly useful tool to probe these mechanisms. We therefore endeavor to carry out direct numerical simulations of nano-void growth in Magnesium using the HotQC method [19–21]. HotQC is a multiscale methodology that provides a systematic coarse-graining strategy for long-term atomistic simulation including both heat and mass transport in solids. This framework combines three key ideas—the maximum entropy (Max-Ent) principle [22], mean field approximation theory and discrete kinetic laws—to extend the zero-temperature quasi-continuum (QC) methodology [23] to study the non-equilibrium finite temperature behavior of atomistic systems with spatial and temporal multi-resolution. A brief overview of this method is now presented for the special case where mass transport is neglected; a detailed discussion of the general case can be found in [19, 21].
We begin by considering a system consisting of $N$ identical particles. Let $\mathbf{q}_i = (q_{i1}, q_{i2}, q_{i3})$ and $\mathbf{p}_i = (p_{i1}, p_{i2}, p_{i3})$ ($i = 1, ..., N$) denote the instantaneous position and momentum of the $i$th particle. The microscopic state of the system is characterized by positions $\{\mathbf{q}\} = (\mathbf{q}_i)_{i=1}^N$ and momenta $\{\mathbf{p}\} = (\mathbf{p}_i)_{i=1}^N$. Denoting the probability density function (pdf) over the phase space as $\rho(\{\mathbf{q}\}, \{\mathbf{p}\})$, the expected/macroscopic value of an observable quantity $A(\{\mathbf{q}\}, \{\mathbf{p}\})$ is obtained using the well known phase average in classical statistical mechanics as

$$
(A) = \frac{1}{h^{3N}} \int_{(1)} A(\{\mathbf{q}\}, \{\mathbf{p}\}) \rho(\{\mathbf{q}\}, \{\mathbf{p}\}) d\mathbf{q} d\mathbf{p}, \quad d\mathbf{q} d\mathbf{p} = \prod_{i=1}^N \prod_{j=1}^3 dq_i dp_j,
$$

where $\Gamma = (\mathbb{R}^{3N} \times \mathbb{R}^{3N})$ is the phase space.

In the HotQC method, the maximum entropy principle is used to choose the pdf such that the information entropy is maximized subject to local constraints; in this case the expected value of the atomic positions, momenta and local energy are constrained for each atom, that is $\langle \mathbf{q}_i \rangle = \mathbf{q}_i$, $\langle \mathbf{p}_i \rangle = \mathbf{p}_i$, and $\langle h_i \rangle = e_i$ respectively. Under these constraints the pdf is obtained as

$$
\rho = \frac{1}{\Xi} \exp^{-\{\beta\|h\}} \quad \text{(2)}
$$

where

$$
\Xi = \frac{1}{h^{3N}} \int_{(1)} \exp^{-\{\beta\|h\}} d\mathbf{q} d\mathbf{p} \quad \text{(3)}
$$

is the partition function of the system, $\{\beta\}$ is the array of reciprocal atomic temperatures defined as $\beta_i = 1/k_B T_i$, $k_B$ is the Boltzmann constant and $T_i$ is the local atomic temperature. Defining the canonical free entropy as

$$
S(\{\mathbf{q}\}, \{\mathbf{p}\}, \{\beta\}) = k_B \log \Xi, \quad \text{(4)}
$$

the governing equations for the thermodynamic system away from equilibrium are postulated along the lines of Hamilton’s equations using the relations

$$
\frac{d\mathbf{p}_i}{dt} = -\frac{\partial H}{\partial \mathbf{q}_i}, \quad \text{(5)}
$$

$$
\frac{d\mathbf{q}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \text{(6)}
$$

$$
H = \sum_{i=1}^N e_i = -\sum_{i=1}^N \frac{1}{k_B} \frac{\partial S}{\partial \beta_i} \quad \text{(7)}
$$

In order to close the system of equations, additional discrete kinematic equations for the evolution of the atomic temperatures need to be introduced. The kinematic equations used in this work describe the particle-wise evolution of the entropy due to heat diffusion according to the relation

$$
\dot{S}_i = \frac{\kappa}{T_i} \Delta \log \left( \frac{T_i}{T_0} \right) \quad \text{(8)}
$$

where $\Delta$ is the discrete Laplace operator evaluated at atom $i$, $T_0$ is the reference absolute temperature and $\kappa$ is an empirical thermal conductivity ($\kappa = 152 \text{ W} (\text{m} \cdot \text{K})^{-1}$ taken from...
macroscopic measurements of bulk Mg [24]). In the calculations presented here, we define the local Laplacian simply by means of an auxiliary finite-element interpolation based on a triangulation of the atomic positions, as described below. The resulting set of equations provide a framework to study non-equilibrium thermodynamics at the atomistic scale.

The aforementioned system of equations can be solved in an explicit way, i.e. by integrating the equations of motion. However, the highly coupled pdf is not computable for very large systems and hence suitable approximations are needed. The HotQC method uses the Gibbs–Bogoliubov inequality in the context of mean field approximations to compute a mean-field canonical free entropy. In this work a family of local trial Hamiltonians corresponding to the representation of each atom as a harmonic oscillator about its mean lattice position is used. The local trial Hamiltonians are thus parametrized by one parameter per atom—the frequency of vibration $\omega_i$. The mean field approximation yields the following Hamilton’s equations in terms of the mesoscopic variables $\{q\}$, $\{p\}$ and $\{\omega\}$,

$$\dot{q}_i = \frac{p_i}{m_i}$$  \hspace{1cm} (9)

$$\dot{p}_i = -\frac{\partial}{\partial q} \sum_{j=1}^{N} (V_j)_0,$$  \hspace{1cm} (10)

$$\frac{\partial}{\partial \omega_i} \sum_{j=1}^{N} \beta_i (V_j)_0 + \frac{3}{\omega_i} = 0,$$  \hspace{1cm} (11)

$$e_i = \frac{|\mathbf{p}_i|^2}{2m_i} + (V_i)_0 + \frac{\partial}{\partial \beta_i} \sum_{j=1}^{N} \beta_j (V_j)_0 + \frac{3}{\beta_i}.$$  \hspace{1cm} (12)

These equations define the evolution of the system in terms of the mesoscopic variables $\{q\}$, $\{p\}$, supplemented by an additional equation that dictates the optimal choice of the mean field parameters $\{\omega\}$.

A crucial feature of the mesoscopic variables previously introduced is that they are amenable to spatial coarse-graining by means of the quasi-continuum framework, since the thermal vibrations are integrated out in the statistical formulation. Thus, using the quasi-continuum method, the mean positions of the atoms are coarse-grained using a finite element triangulation $T_{QC}$ over a set of representative atoms (repatoms). The set of repatoms, $L_{QC}$, is a subset of the atoms in the crystals $L$, and is chosen such that it is dense (i.e. fully atomistic) near defects and is gradually coarsened away from the defect core. The atomic fields are then interpolated using the shape functions provided by the triangulation $T_{QC}$. Therefore, atomic positions, temperature and frequencies for atoms that do not belong to the triangulation are interpolated as

$$q_i = \sum_{j \in L_{QC}} \Gamma_i q_j,$$  \hspace{1cm} (13)

$$\omega_i = \sum_{j \in L_{QC}} \Gamma_i \omega_j.$$  \hspace{1cm} (14)
where $i$ runs over each atom in the system and $\Gamma_{ij}$ are the shape functions associated with the finite element triangulation $\mathcal{Q}_C^T$. Finally, by virtue of the QC-interpolation, energy and forces can be computed using the cluster summation rules proposed by Knap and Ortiz [25].

**2.2. Simulation set up**

In all our calculations, we use the embedded atom model (EAM) proposed by Liu et al [26] to model the interatomic potential for Mg. The external dimensions of the crystal used in the simulations are $128a_0 \times 128a_0 \times 128c_0$ (containing 4, 194, 304 atoms), unless otherwise specified. $a_0 = 3.20$ Å and $c_0 = 5.21$ Å are the unit cell lattice parameters of the HCP structure, chosen such so as to minimize the free energy at $T_0 = 300$ K. An initial minimization is carried out using adaptive dynamic relaxation [27] by allowing isothermal expansion of the computational cell. A fully atomic zone of size $16a_0 \times 16a_0 \times 16c_0$ is used in the initial mesh,

**Table 1.** Critical volumetric strain for dislocation emission ($\epsilon_c$), peak stress ($\sigma_p$) and dislocation velocity along the basal plane ($v_d$) for different strain rates ($\dot{\epsilon}$) for a Mg single crystal of dimension $128a_0 \times 128a_0 \times 128c_0$ (43 nm$^3$) with a nano-void of diameter $\Phi = 3.84$ nm at $T_0 = 300$ K.

<table>
<thead>
<tr>
<th>$\dot{\epsilon}$ (s$^{-1}$)</th>
<th>$10^3$</th>
<th>$10^6$</th>
<th>$10^7$</th>
<th>$10^8$</th>
<th>$10^9$</th>
<th>$10^{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon_c$ (%)</td>
<td>16.5</td>
<td>16.5</td>
<td>17.5</td>
<td>19.0</td>
<td>23.5</td>
<td>25.5</td>
</tr>
<tr>
<td>$\sigma_p$ (GPa)</td>
<td>2.41</td>
<td>2.47</td>
<td>2.57</td>
<td>2.70</td>
<td>3.15</td>
<td>3.85</td>
</tr>
<tr>
<td>$v_d$ (m s$^{-1}$)</td>
<td>15</td>
<td>25</td>
<td>100</td>
<td>295</td>
<td>310</td>
<td>312</td>
</tr>
</tbody>
</table>

\[ T_i = \sum_{j \in \mathcal{Q}_C} \Gamma_{ij} T_j \tag{15} \]

Figure 1. Virial stress for different strain rates for a Mg single crystal of dimensions $128a_0 \times 128a_0 \times 128c_0$ (43 nm$^3$) with a nano-void of diameter $\Phi = 3.84$ nm at $T_0 = 300$ K.

Table 1. Critical volumetric strain for dislocation emission ($\epsilon_c$), peak stress ($\sigma_p$) and dislocation velocity along the basal plane ($v_d$) for different strain rates ($\dot{\epsilon}$) for a Mg single crystal of dimension $128a_0 \times 128a_0 \times 128c_0$ (43 nm$^3$) with a nano-void of diameter $\Phi = 3.84$ nm at $T_0 = 300$ K.
and the atoms are coarsened rapidly away from this zone resulting in around 30 000 representative atoms. In the center of the fully atomic zone, an approximately spherical nano-void of diameter $\Phi$ is created by removing atoms from the mesh. Unless otherwise specified, the diameter of the nano-void shown in the figures is $\Phi = 12a_0 = 3.84$ nm. A finite element mesh is then constructed using Delaunay triangulation on the representative atoms. This mesh supports adaptive mesh refinement using the distortion of the elements as the critical parameter for remeshing [28].

At each time step a homogeneous deformation gradient $\mathbf{F} = (1 + \lambda)\mathbf{I}$ (where $\mathbf{I}$ is the $3 \times 3$ identity matrix) is applied to the sample to generate a triaxial deformation to simulate the conditions encountered in spallation. The parameter $\lambda$ is adjusted to obtain the desired strain rate in the simulation (see table 1). Virial stresses are computed according to the methods elaborated in [29] and the stress values reported are obtained using $\sigma = 1/3(\sigma_1 + \sigma_2 + \sigma_3)$ where $\sigma_i$ are components of the principal stress. The volumetric strain is computed using the relation $\epsilon = \Delta V(t)/V_0$ where $\Delta V(t) = V(t) - V_0$ is the increment in the sample volume at a time $t$ with respect to the initial volume $V_0$ at 300 K. All dislocations are visualized with OVITO [30]. The details of the simulations performed at different strain rates are summarized in table 1.

### 3. Results

We start our analysis by describing the evolution of virial stress with volumetric deformation, as illustrated in figure 1 for different strain rates. Figure 1 shows an initial linear elastic regime that extends until a critical volumetric deformation for dislocation emission ($\epsilon_c$, reported in table 1) is reached. Once the volumetric deformation reaches $\epsilon_c$, the void starts the process of cavitation by dislocation emission, increasing in volume at a high rate. At this point dislocations are emitted from the void surface and the virial stress increases with deformation until it reaches $\sigma_p$, the peak stress. After this point the material rapidly fails due to several cracks propagating in the material. Interestingly, no secondary strain-hardening near the void is observed as in other materials like FCC or BCC [31, 32]. This observation is of fundamental importance for the design of new lightweight alloys since, according to our simulations, the spall strength of pure Mg is very low due to this phenomena. Our simulations also show that the evolution of the virial stress for different void sizes is very similar to the one previously described. As can be seen from table 2, the peak stress drops significantly only for large voids ($\Phi \geq 6.0$ nm).

The analysis of dislocations generated by the nano-void surface indicates that under hydrostatic tensile load, dislocations in Mg single crystals have the same topology irrespective of the nano-void size. However, the peak stress values are affected by the nano-void size and it is important to determine what the optimal nano-void and cell sizes are. The results reported in table 2 indicate that the peak stress does not vary significantly for void volume fractions ($\rho = V_{\text{void}}/V_{\text{cell}}$) below 0.01. Similarly, we assessed the influence of the cell size on the peak stress for a nano-void of diameter $\Phi = 3.84$ nm. We carried out four simulations using different cell sizes, i.e. $64a_0 \times 64a_0 \times 64c_0$, $96a_0 \times 96a_0 \times 96c_0$, $128a_0 \times 128a_0 \times 128c_0$ and $192a_0 \times 192a_0 \times 192c_0$. The peak stress values obtained from our simulations are illustrated...
in figure 2. We see that the peak stress becomes insensitive to the cell size when the cell length approaches $128a_0$.

The results obtained by studying the effect of cell size for different nano-void sizes suggest that the simulations carried out with nano-voids of diameter $\Phi = 3.84$ nm and cell size dimensions of $128a_0 \times 128a_0 \times 128c_0$ are sufficient to mitigate the effect of boundaries in the simulations. We therefore use this combination of nano-void diameter and cell size to describe the nature of dislocations near the void surface, peak stress values and dislocation velocities in the remainder of this document.

We proceed to describe in detail the emission of dislocations from the void surface to facilitate an understanding of the mechanism of deformation during nano-void growth under triaxial tensile stress. Our simulations show that the topology of the dislocations emitted from the void surface is always of the same type and therefore, the mechanisms are invariant with respect to strain rate. Consequently, the dislocations shown in the following figures correspond to $\dot{\varepsilon} = 10^5$ s$^{-1}$ unless otherwise specified. The first set of dislocations is emitted from the void surface at a volumetric deformation $\epsilon_v$ (reported in table 1 for various strain rates) and the dislocations are illustrated in figure 3. The dislocation emission occurs at the location of maximum shear stress, viz. the intersection of the void surface and a plane located at $z \approx \pm 0.75R$, where $R = \Phi/2$ is the nano-void radius. The dislocations emitted involve a set of dislocation loops of the type $1/3\langle 1 \bar{1} 00 \rangle \{0001\}$ that glide on the basal plane. As these dislocations evolve and move outside the void, they interact with the nearest dislocations to generate a screw dislocation with Burgers vector $1/3\langle \overline{\Gamma\Gamma20} \rangle \{0001\}$ that glides on the basal plane as well. The reaction is given by:

$$
\frac{1}{3}[1010] + \frac{1}{3}[0110] \rightarrow \frac{1}{3}[\overline{\Gamma\Gamma20}] \tag{16}
$$

In total, twelve edge and screw dislocations are emitted at $z \approx \pm 0.75R$ as depicted in figure 3, where a top view (looking down along the $c$-axis) of both the atomic structure of
the dislocations and a schematic representation of the basal dislocations along with the screw
dislocations that form according to the reaction equation (16) are shown.

After the emission of basal and screw dislocations, a secondary set of $\frac{1}{3}(1\overline{1}00)\langle001\rangle$ prismatic dislocations are emitted from the void surface and are shown in figure 4 by the letter ‘P’. These dislocations glide on the $\langle10\overline{1}0\rangle$ planes (which are perpendicular to the basal plane) and are bounded by the aforementioned basal dislocations. The prismatic dislocations

Figure 3. Dislocations emitted from the void surface for $\epsilon_c$ reported in table 1. Partial shears loops $\frac{1}{3}(1\overline{1}00)\langle001\rangle$ as well as screw type dislocations $\frac{1}{3}(1\overline{1}20)\langle001\rangle$ are observed. Burgers vectors of the dislocations are specified in the figure.

Figure 4. Emission of secondary prismatic loops around the nano-void at $\epsilon = 17\%$ and $\dot{\epsilon} = 10^5$ s$^{-1}$. Perspective view of the nano-void and dislocations with a cut around $z = 0.75R$. Void surface has been indicated, screw dislocations are denoted with the letter S and prismatic dislocations are denoted with P. The screw dislocations push the prismatic loops away from the void surface.
are pushed away from the void surface by two screw dislocations that lie on the basal plane, as indicated in figure 4 by the letter ‘S’. Following an initial interaction of the prismatic dislocations, they subsequently travel away from the void surface without any resistance and without causing any additional strain hardening.

Upon increasing the strain, a final set of dislocations with a \((c+a)\) Burgers vector is emitted from the top of the void surface. The \((c+a)\) dislocations glide along the pyramidal-I plane and are only observed above the peak stress (\(\geq 2.4\) GPa) and serve to release the high stress on the void surface. It is noted that prior to the emission of \((c+a)\) dislocations, the void volume primarily grows along the basal plane with dimension along the \(c\)-axis being nearly constant. The high stress near the core of the \((c+a)\) dislocation induces a separation of the atoms along the glide plane and initiates the propagation of multiple cracks that rapidly result in a failure of the specimen. Along with the cracks opening in the material, several basal dislocations are further emitted. The set of dislocations towards the end of the simulation is illustrated in figure 5.

The previous description of dislocation emission and crack formation with deformation is of high relevance to the design of new lightweight materials under dynamic loads. The very low resistance to slip along the basal plane in Mg promotes an early onset of plastic deformation near the void, thus greatly reducing the critical stress for dislocation emission in comparison with other materials. Along with the onset of plastic deformation, the void experiences an anisotropic change of shape and volume. This in turn produces a high concentration of stresses on the nano-void surface and initiates the emission of multiple cracks in the materials, resulting in dynamic failure. Furthermore, our simulations do not show a secondary strain hardening regime near the void, unlike materials like Al or Cu where sessile and glissile dislocations interact to produce additional strain hardening near the void [28, 31]. This lack of strain hardening is due to the fact that basal and prismatic dislocations can travel away from
the void without any interaction with non-basal dislocations. Although pyramidal dislocations can be emitted and can provide the desired interaction between slip systems on the basal plane and along the \( c \)-axis, the Peierls barrier associated with them is very large, thus limiting the emission and glide of this type of dislocation [6–8]. This overall behavior leads to the emission of two, almost independent, sets of dislocations, and hence very small strain hardening.

In FCC materials, secondary strain hardening has important consequences for dynamic behavior since it increases the peak stress reached in the material, reduces the motion of dislocations and helps to dissipate some of the energy coming from the shock load. In contrast, for Mg, the unconventional lack of secondary strain hardening is thus of fundamental importance because it limits the peak stress, and ultimately, the spall strength of Mg.

We present next a parametric study of the evolution of the peak stress and the dislocation velocity as a function of the strain rate. We carried out simulations at strain rates in the range \( \dot{\varepsilon} = 10^5 - 10^9 \text{ s}^{-1} \). Figure 6 shows the evolution of the peak stress and the dislocation velocity along the basal plane as a function of the strain rate. The dislocation velocities are measured with the method described in [28]. We observe that for moderate strain rates \( \dot{\varepsilon} = 10^5 - 10^7 \text{ s}^{-1} \) an asymptotic behavior is reached for the peak stress while for very high strain rates \( \dot{\varepsilon} = 10^8 - 10^9 \text{ s}^{-1} \) it increases very quickly. Similarly, figure 6 clearly shows a transition in the dislocation velocity from moderate to very high strain rates. This transition is significant since the dislocation velocity increases from 15 to 312 m s\(^{-1}\). The behavior at both ends is asymptotic. The critical role of strain rates resulting in two distinct trends in dynamic failure, as observed in the behavior of the peak stress and dislocation velocity with strain rate, is a clear evidence of the nonlinear response of the material under dynamic loads.

We finally describe the coupled thermo-mechanical response of the material by analyzing the temperature evolution of the sample. Figure 7 shows the evolution of the temperature of an atom on the void surface for different strain rates. For very high strain rates, the thermoelastic response of the material is characterized by a steady change in the temperature until the cavitation point. Once dislocations are emitted from the void surface, the local atomic temperature experiences a nonlinear transition due to the conversion of plastic work into thermal energy. This exchange of energy is highly localized on atoms near the dislocation cores and void.

Figure 6. Evolution of the peak stress and dislocation velocity along the basal plane for various strain rates. There is a clear increment in the peak stress for strain rates larger than \( 10^7 \text{ s}^{-1} \). A transition in dislocation velocity around \( \dot{\varepsilon} = 10^7 \text{ s}^{-1} \) with a double asymptotic behavior is observed.
surface and is therefore heterogeneous along the computational cell, resulting in sharp spatial gradients in the temperature field as shown in figure 7 (inset). We also observe that the evolution of the temperature field is less pronounced as the strain rate decreases (i.e. $\dot{\varepsilon} < 10^8 \text{s}^{-1}$).

As a limiting case, the simulation carried out at $\dot{\varepsilon} = 10^5 \text{s}^{-1}$ shows an isothermal behavior. The corresponding thermodynamic transition, which is called adiabatic-to-isothermal transition is a consequence of the coupled thermo-mechanical response of the material that is modeled by the non-equilibrium physics encoded in the atomistic heat conduction model and the spatial and temporal coarse-graining framework based on the HotQC method.

4. Comparison with experiments

Spall experiments of Mg and Mg-alloys have been carried out in the past by many researchers. Schimdt et al [33] studied the spall strength of Mg-alloys (AZ-31B-H24) and reported a spall strength of about 1.5 GPa for specimens where incipient spallation was observed. Kanel et al [34] studied the spall properties of Mg at different temperatures using specimens which contained 99.95 wt% of Mg (we refer to this data as Mg95 in the following) and reported a spall strength between 0.77–1.0 GPa for strain rates between $10^5$ to $4 \times 10^5 \text{s}^{-1}$ respectively, at $T = 300 \text{K}$. Garkushin et al [35] studied the spall strength spall strength of Ma2 Mg alloy (93.7% Mg, 4.36% Al, 1.34% Zn and 0.39% Mn). They reported a spall strength in the range of 1.05–1.33 GPa with strain rates in the range of $10^5$–$10^6 \text{s}^{-1}$ respectively, at $T = 300 \text{K}$. More recently, Kanel et al [36] investigated the spall strength of high purity Mg single crystals (99.99% Mg by weight) and the effect of the crystal orientation and reported a spall strength between 1.19–1.64 GPa for strain rates in the neighborhood of $2 \times 10^5$ at $T = 300 \text{K}$.

It bears emphasis that extrapolating the results obtained from our numerical simulations to experimental measurement of spall is not entirely reliable. Magnesium often contains precipitates, and fractography reveals that the incipient nucleation of voids during spallation
occurs at the location of precipitates. This is also consistent with the dependence of spall on the purity of magnesium. Other defects like grain boundaries and twin boundaries may also act as spall nucleation sites. Therefore, the peak stress obtained in our simulations should be interpreted as an upper bound of the spall strength of Mg single crystals. Figure 8 shows a plot where experimental results obtained in the previous works have been gathered.

We have also included the peak stress values obtained for a wide of strain rates and void sizes between $10^5$–$10^8$ s$^{-1}$ and $\Phi = 2.24$–7.36 nm respectively. For experiments carried out in single crystal Mg at strain rates of $10^5$ s$^{-1}$ the spall strength is of the order of 1.25–1.64 GPa depending of the orientation, while for our simulations the peak stress is in the range of 1.92–2.41 GPa depending of the initial size of the prescribed nano-void. Using the mean values of these two ranges we see that the difference is spall strength between spall experiments of single crystals and our simulations is about 0.72 GPa. Considering the fact that the only input in our model is the interatomic potential and that the simple set up of our simulation is a highly idealized representation of an actual single crystal, we find that the agreement with experiments is quite remarkable in spite of the fact that many factors that might affect spall strength are not taken into account.

The remarkably good agreement between the predictions of spall strength using our simulations and experimental data suggests that the mechanisms observed in our simulations play a crucial role in spallation. On the other hand, the comparison with experiments also tells us that there might be additional mechanisms not taken into account in our simulations that affect the spall behavior as well. The insights provided by our multiscale simulations thus provide a means to understand, manipulate and ultimately control spall in Magnesium, thereby aiding in the design of new and better alloys with superior properties. In particular, the effect of alloying elements on the spall strength of Mg alloys is currently being investigated by the authors.

Figure 8. Experimental spall strength for Mg and Mg alloys in single and poly-crystals and peak stress obtained from our simulations for a wide range of strain rates. Mg95, Ma2 and single crystal data (SC) are values reported by Kanel et al [33], Garkushin et al [34] and Kanel et al [35] respectively. We also show the peak stress obtained from our simulations for comparison.
5. Conclusions

In summary, we studied the process of nano-void cavitation by dislocation emission in pure Magnesium for strain rates ranging from $\dot{\varepsilon} = 10^5$ to $10^{10}$ s$^{-1}$, for various nano-void sizes at 300 K using the HotQC method. Our simulations show a conspicuous absence of secondary strain hardening near the nano-void that greatly limits the peak stress reached during the simulation and ultimately, the spall strength of Mg. The lack of secondary hardening is due to the inability of HCP materials to produce the desired interaction between basal and prismatic dislocations on the one hand, and pyramidal dislocations on the other.

Our analysis also shows that there is a transition in both the dislocation velocity and peak stress when the strain rate changes from $\dot{\varepsilon} = 10^5$ to $10^{10}$ s$^{-1}$. In the case of the dislocation velocities, the behavior is asymptotic at both ends, with a rate dependent behavior at moderate strain rates. For the peak stress, dynamic effects become small at moderate strain rates and therefore, the peak stress is almost constant in the range $\dot{\varepsilon} = 10^5$–$10^7$ s$^{-1}$. The evolution of temperature with strain rate is also studied. The temperature field is strongly dependent on the strain rate, changing the behavior of the material from adiabatic-to-isothermal from very high to moderate strain rates. In general, our simulations reveal the emergence of complex temperature fields that are tightly coupled and strongly influenced by the evolution of plasticity in the material. This coupling clearly evinces the rate sensitivity of the dynamic response of the material under extreme conditions.

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References

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