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Nanovoid failure in Magnesium under dynamic loads

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ABSTRACT

The dynamic behavior of Magnesium (Mg) single crystals containing nano-sized voids and the mechanisms responsible for failure under different loading conditions are studied by means of Molecular Dynamics (MD) simulations. Our study reveals that the response is highly anisotropic leading to a brittle to ductile transition in the failure modes under different load orientations. This transition is accompanied by different mechanisms of deformation and is associated with the anisotropic Hexagonal Close Packed (HCP) lattice structure of Mg and the associated barrier for dislocation motion. Remarkably, brittle failure is observed when external loads produce a high stress triaxiality while the response is more ductile when the stress triaxiality decreases. The fundamental mechanisms observed in the simulations, therefore, explain the low spall strength of Mg and suggest the possibility of manipulating some mechanisms to increase ductility and spall strength of new lightweight Mg alloys.

1. Introduction

Magnesium (Mg), the lightest of all metallic materials and one of the most abundant elements in the earth's crust, offers tremendous opportunities for modern lightweight applications in engineering. Its low density and high specific strength (material's strength divided by its density) make Mg and its alloys recognized alternatives to iron and aluminum based-alloys to satisfy the strong demand of weight reduction. However, Mg and its alloys have poor mechanical properties such as ductility and low yield strength, which hinder widespread industrial use of these materials [1–3].

This is largely a consequence of the HCP lattice structure of Mg. A key characteristic of the HCP lattice structure is that only four independent slip systems are available to produce plastic deformation, which is in contrast with FCC and BCC lattice structures where five independent slip systems are available [4]. Additionally, in Mg, the basal and prismatic slip systems are usually easily activated whereas the critical stress for dislocation glide in the pyramidal systems is at least one order of magnitude higher than in the basal plane [5–7]. This anisotropy in the slip systems results in a profusion of twinning that is activated in order to deform along the [0001]- crystallographic direction [8].

In this work, numerical simulations are performed to understand the deformation mechanisms operative in Mg during dynamic failure. Dynamic failure is a complex phenomenon that occurs when materials are subject to high velocity impacts and is characterized by a strongly coupled thermo-mechanical evolution of nanovoids. Under these conditions, materials usually fail by spallation [9,10]. The spall failure happens due to the high tensile stresses reached in the spall plane, where nano-sized voids are quickly nucleated, leading to nanovoid growth and coalescence, and eventually, the propagation of cracks in the specimens [11–13]. Due to the complex mechanisms that have place during dynamic failure and spallation, the experimental characterization is extremely challenging and restricted only to indirect measures, i.e., free surface velocity or *post-mortem* examination of specimens.

In spite of the limitations of current experimental techniques to study nanovoid growth under dynamic loads, numerical simulations using MD provide a highly useful tool to probe these mechanisms. The main goal of this work is to shed light on the mechanisms that dominate dynamic failure mode by nanovoid growth and thereby, provide insights that can be used to inform the design of new Mg-based alloys. MD has been used in the past by many researchers to predict nanovoid growth in different materials including FCC [14–21] and BCC [22–24] materials, to mention but a few.

While the literature is broad on either FCC or BCC materials, there is a clear lack of bibliography for nanovoid cavitation in HCP materials. In a recent study, Ponga et al. [25] have studied the dynamic behavior of nanovoids in Mg using the HotQC method and analyzed the mechanisms of deformation for hydrostatic tensile

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loads and the transition regimes observed for moderate to high strain rates. While the study of Ponga et al. [25] provides valuable fundamental understanding in the dynamic behavior of Mg under hydrostatic tensile loads, the key mechanisms involved in the dynamic failure under different load orientations are not well understood and remain an open question. This work complements and expands the aforementioned study to multiple load conditions in an effort to answer some of these questions. Therefore, we seek to understand the mechanisms that have place during the dynamic failure of Mg under five different loading conditions using MD simulations. These loading conditions are used in order to activate different slip systems to understand the main mechanisms active during nanovoid failure.

One of the most critical aspects of MD simulations is the choice of the interatomic potential. It is well known that the mechanisms of deformation may change from one potential to another during nanovoid growth [21] and for that reason it is essential to assess the fidelity of the results and mechanisms of deformation for different interatomic potentials. Thus, an ancillary objective of this work is to assess the fidelity of the mechanisms of deformation using different potentials for Mg. This task is not trivial since there is no standard or routine benchmark test for interatomic potentials.

This issue has been investigated by many researchers in recent years. Yasi et al. [5] have studied the basal dislocations core in Mg using two Embedded Atom Method (EAM) [26] interatomic potentials proposed by Liu et al. [27] and Sun et al. [28], respectively. More recently, Ghazisaeidi et al. [29] have studied the edge and screw dislocation cores in Mg with the aforementioned EAM potentials developed by Liu et al. and Sun et al. and a newly second nearest neighbors Modified Embedded Atom Method (2NN-MEAM) [30,31] proposed by Kim et al. [32]. They have concluded that neither three potentials can capture all the details observed with methods based on the Density Functional Theory. Motivated by these issues, Wu et al. [33] have developed an improved and promising Modified Embedded Atom Method (MEAM) based on the original potential of Kim et al. [32].

It is important, therefore, to provide tools for future works where one can select the adequate interatomic potential for the study of a particular problem of interest. Hence, we endeavor to assess the efficiency and fidelity of the mechanisms of void growth and dislocation emission for two different interatomic potentials. In addition to test the potentials in single dislocations set up as in the previous works, we benchmark the potentials according to the peak stress, dislocations topology, and critical strain for dislocation emission under different loading conditions. Remarkably, only minor differences are encountered and the overall behavior is essentially the same for the two potentials.

The manuscript is organized as follows. Section 2 explains the methodology used in the simulations carried out in this work. Section 3 presents the results obtained for five different loading cases. For all cases, the virial stress and the Von Mises equivalent stress *vs.* strain evolution, dislocations density, emission, topology, and velocities are studied. For the hydrostatic tensile load, a meticulous analysis is provided including the effect of void size, cell size, temperature, and dislocation velocities. Section 4 presents a discussion of the main results obtained in this work. Finally, the document is summarized with the main conclusions.

2. Methodology

2.1. Nanovoid simulations

Numerical simulations of nanovoid cavitation under different tensile loads in pure Mg single crystals are carried out using MD at a range of strain rates between $\dot{\varepsilon} = 10^7 - 10^{10}\ \mathrm{s}^{-1}$. All simulations are performed with the LAMMPS code [34] and the material (Mg) is modeled with two different interatomic potentials developed by Sun et al. [28] and Wu et al. [33]. We will refer these interatomic potentials in the remaining of this document as EAM and MEAM potentials, respectively. The first one is based on the *embedded atom method* [26] while the second one is based on the *second nearest neighbors modified embedded atom method* (2NN-MEAM) [30]. These potentials are systematically used to analyze the fidelity of the mechanisms of deformation in Mg.

A rectangular parallelepiped of dimensions $l_x \times l_y \times l_z$ is used to generate a Mg single crystal. The HCP lattice structure is generated with $a_0 = 0.319$ nm and $\frac{c_0}{a_0} = 1.626$, where a_0 is the lattice constant on the basal plane and $\frac{c_0}{a_0}$ is the ratio between the lattice constants in the $[0001]$ direction and the basal plane at 0 K, respectively. Unless otherwise specified, the external dimensions of the computational cell are $l_x = 38$ nm, $l_y = 68$ nm and $l_z = 68$ nm which correspond to a selection of 120^3 HCP units cells containing approximately 7 million atoms. The crystals are constructed in such a way that the crystallographic directions $[2\bar{1}\bar{1}0]$, $[01\bar{1}0]$ and $[0001]$ of the HCP lattice structure are aligned with the $x-$, $y-$ and $z-$ axes of the computational box, respectively. Then, an initial void of diameter ϕ is generated by removing atoms from the center of the crystal. Unless otherwise specified $\phi = 20a_0 = 6.3$ nm. Finally, periodic boundary conditions are used in all simulations containing nanovoids.

Unless otherwise specified, the temperature of the computational cell is initialized at a constant value of T = 300 K. The initial configuration is relaxed by integrating the equations of motion for 40 ps without applying any load. During this relaxation process the crystal is allowed to expand and/or contract independently in each orthogonal direction allowing to minimize the energy and the pressure of the computational cell using an NPT ensemble with a Nosé-Hoover thermostat and a time step of $\Delta t = 5$ fs. Once the initial relaxation is completed, the individual components of the stress tensor are zero within ±5 MPa.

After the initial relaxation is achieved, a controlled displacement deformation is applied to the simulation cell by using a homogeneous deformation gradient $\mathbf{F}$ at each time step. Let $\mathbf{x}_n^i$ be the position vector for an atom i at the time step n and $\mathbf{F}$ be the deformation gradient, thus the new position of the atom i at the time step $n+1$ is computed as $\mathbf{x}_{n+1}^i = \mathbf{F}\mathbf{x}_n^i$. The deformation gradient is

$$\mathrm{F} = \begin{pmatrix} 1 + n_1\dot{\varepsilon}\Delta t & 0 & 0 \\ 0 & 1 + n_2\dot{\varepsilon}\Delta t & 0 \\ 0 & 0 & 1 + n_3\dot{\varepsilon}\Delta t \end{pmatrix} \tag{1}$$

where $\boldsymbol{n} = \{n_1, n_2, n_3\}$ is a vector whose components are either one or zero, $\dot{\varepsilon}$ is the strain rate and Δt is the time step. The deformation gradient $\mathbf{F}$ is changed for each loading case by selecting different choices of $\boldsymbol{n}$. We change the deformation gradient in order to activate different slip systems and understand the main

Table 1
Selected values of $\boldsymbol{n}$ for different loading cases.

Load	$[2\bar{1}\bar{1}0]$	$[1\bar{1}00]$	$[0001]$
Case 1	1	1	1
Case 2	1	0	1
Case 3	1	1	0
Case 4	1	0	0
Case 5	0	0	1