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Analytical model for estimating calcium solution strengthening in single-crystal Mg-Ca alloys at finite temperatures

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Keywords

Molecular dynamics, Magnesium alloy, Solid solution strengthening, Edge dislocation, Critical resolved shear stress

Abstract

Mg is the lightest structural metal and a suitable replacement for heavy steel and Al alloys. However, Mg exhibits poor plastic formability at room temperature, and the strength of conventional Mg alloys is less than that of most Al alloys. Its low formability at room temperature is attributed to the lack of slip systems because of the extremely large gap in the critical resolved shear stress (CRSS) between the lowest basal system and the other slip and twin systems. This low CRSS of the basal slip usually limits the strength of Mg alloys. Therefore, strengthening the basal slip is important to improve the strength and deformability of Mg alloys and enhance their ductility. In this study, we construct an analytical model for predicting the CRSS in single-crystal Mg–Ca alloys at finite temperatures by quantitatively investigating the CRSS for the $\langle a \rangle$ dislocation gliding on the basal plane at temperatures from 1 to 500 K through molecular-dynamics computations. The prediction results agree well with our simulation results and the micropillar compression test results of Mg–0.3at.%Ca and Mg–0.6at.%Ca alloys at room temperature.

1. Introduction

Mg is the lightest structural metal, whose density is 66% of that of Al and 25% of that of steel. Mg alloys have high stiffness-to-weight and strength-to-weight ratios, and are readily available and easily extractable, as Mg accounts for 2.7% of the Earth's crust, and can be produced at high purities on a large scale [1]. With the increasing demand for energy saving and environmental protection, Mg alloys have attracted interest as candidates for lightweight applications in the field of transportation, aerospace, computers, communication, and consumer electronic products [2, 3, 4]. However, Mg alloys have relatively low strength and ductility at room temperature [5, 6] and exhibit poor strengthening with the conventional thermal aging techniques, compared to Al alloys.

Unlike Al, which has a face-centered-cubic crystallographic structure with 12 equivalent slip systems, Mg has a hexagonal-close-packed structure with only several slip variants: basal $\langle a \rangle$, prismatic $\langle a \rangle$, pyramidal $\langle a \rangle$, and pyramidal $\langle c+a \rangle$ (pyramidal I & II) [7]. These distinct slip systems have different critical resolved shear stress (CRSS) values, and the CRSS ratio of nonbasal to basal slip systems is 40–100 for single crystals and 4–6 for pure Mg polycrystals [8, 9]. Therefore, it is difficult to activate the possible nonbasal slip modes, and the strength and plastic deformation of Mg alloys at low temperatures are substantially affected by the basal slip. In other words, approaches that increase the CRSS of the basal slip can help strengthen Mg alloys. Solute atoms, solute clusters, and nanoscale precipitates can improve the strength of Mg alloys by pinning the motion of dislocations [10]. In this work, we focus on the solid-solution enhancement of the strength of Mg alloys and the corresponding decrease in the CRSS gap between the basal and other slip systems, for achieving the desired formability.

The addition of rare earth (RE) elements such as Y and Gd is an effective means to improve the strength of Mg alloys [11, 12]. However, because Mg–RE alloys are not commercially desirable, the development of RE-free Mg alloys is an active area of research [13, 14]. To design RE-free Mg alloys with performances similar to or better than that of Mg–Y alloys, Sandlöbes et al. [15] developed a quantum-mechanically derived design map that screened solid-solution combinations with electronic bonding, structure, and volume descriptors similar to that of Mg–Y alloys. The combination of Al and Ca was the only pair that remained after filtering 2850 solute pairs. They

synthesized a Mg–1wt.%Al–0.1wt.%Ca alloy that was over four times more ductile and 40% stronger than pure Mg. However, a Mg–1wt.%Al–0.3wt.%Ca alloy exhibited much less ductility than pure Mg. Thus, the Ca content in Mg alloys can substantially change the alloy properties; with a larger atomic size than Y, Ca is considered having the ability to strengthen the solution in Mg. However, most studies have investigated the improvements in ductility only [16, 17, 18]; there has been no quantitative investigation on the effects of Ca content in Mg alloys. According to the strengthening design map developed using the first-principles data in [19], Ca might have a more substantial strengthening effect than Y. However, the effect of Ca addition on strengthening is still not apparent.

Although the experimental data on Mg–Ca alloys are insufficient, Akhtar and Teghtsoonian [20] found that the CRSS for the basal slip in Mg–Zn alloys increased proportional to the square root of the solute concentration at temperatures less than room temperature. However, they also reported that the CRSS of Mg alloys at temperatures above 295 K could be best described by a c^n relationship, where c is the atomic fraction of the solute and n is equal to 2/3 [21]. The solute strengthening exponent n was predicted to be 1/2 using the Butt–Feltham model [22] and 2/3 using the Labusch model [23]. However, Vanderplanken and Deruyttere [24] indicated that the CRSS had a linear relationship with c in Mg–Sn alloys at room temperature; i.e., n equaled 1. Therefore, the relationship between CRSS and the solute concentration remains unclear. Moreover, there have been no quantitative computational studies on the effect of Ca addition on the strengthening of diluted Mg alloys, including the temperature effect. Thus, in this study, we investigate the strengthening effect of Ca by quantitatively studying the CRSS of the edge dislocation slip on the basal plane. We also aim to develop an analytical model that can estimate the Ca solute-strengthening effect by comparing and verifying with experimental data.

2. Simulation methodology

Molecular dynamics (MD) simulations were performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [25], an open-source platform developed by Sandia National Laboratories. The Mg–Ca modified embedded-atom method (MEAM) potential developed by Kim et al. [26] was used in our simulations. The Mg–Ca potential is the second-nearest-neighbor (2NN) MEAM

interatomic potential, which reproduces several basic material properties. By using this potential, Kim et al. [27] revealed that Ca atoms had stronger dislocation binding tendencies on basal $\langle a \rangle$ slip planes than on nonbasal $\langle c+a \rangle$ slip planes, consistent with the experimental results obtained in [15].

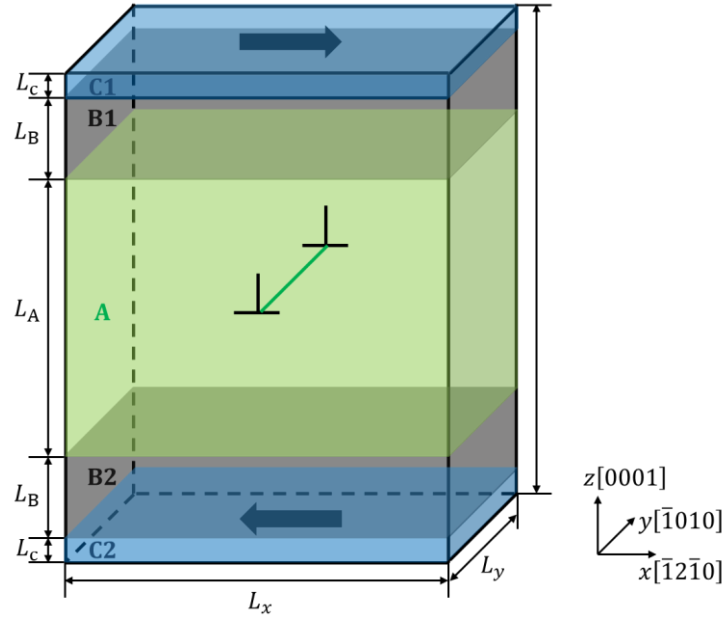


Fig. 1. Schematic of the initial configuration of a system containing an edge dislocation denoted by “ $\perp$ ” in the center of a box. Shear loading with a constant strain rate is superimposed on the atoms in the C1 and C2 blocks.

Single-crystal hexagonal-close-packed Mg-based models with initial orientations of x : $[\bar{1}2\bar{1}0]$, y : $[\bar{1}010]$, and z : $[0001]$ were considered in this study. Following the work of Yi et al. [28], an edge dislocation was inserted by joining two half-crystals on the (0001) plane, with the top half of the crystal containing one additional $(\bar{1}2\bar{1}0)$ atomic plane than the bottom half. Fig. 1 shows an edge dislocation at the center, lying on the slip plane. To examine the finite-size effect, MD simulations were performed using different simulation cells of lengths $L_x = 20\text{--}40$ nm, $L_y = 5\text{--}10$ nm, and $L_z = 25\text{--}75$ nm. We found that the CRSS values of these different simulation cells did not change substantially when the box size was larger than $20\text{ nm} \times 5\text{ nm} \times 50\text{ nm}$. Therefore, all calculations in this study were performed using the minimum box size. The used model corresponded to a dislocation density of $\rho \approx 10^{15}\text{ m}^{-2}$. Three computational steps were performed in each shear deformation calculation. First, the conjugate gradient

algorithm was used to minimize the system energy with an energy tolerance of 10^{-16} eV and force tolerance of 10^{-12} eV $\text{\AA}^{-1}$, to obtain a stable structure. Then, the minimized system was thermally equilibrated in an isothermal–isobaric ensemble (NPT ensemble) with a Nose–Hoover thermostat/barostat [29] at a time step of 1 fs. The hydrostatic pressure was set as zero. Periodic boundary conditions (BCs) were selected along the x , y , and z -axes until the equilibration was complete. Once the equilibrium configuration was achieved, the dynamically relaxed system was subjected to shear deformation.

Periodic BCs were applied to both the x and y -axes to enable simulations of infinitely long dislocations gliding over an arbitrary distance. Flexible BCs [30], which could reduce nonphysical stress oscillations, were applied to the C1 and C2 blocks. The flexible BCs could reduce the mismatch between the motions of the surface region and dislocations by enabling atomic relaxation in C1 and C2 along the x , y , and z directions. To apply the flexible BCs, the average atomic velocities and forces were first calculated along the x direction in C1 and C2. Subsequently, opposite-signed average velocities and atomic forces were added to all atoms in C1 and C2 to set the average velocities and forces in C1 and C2 to zero. Next, a constant velocity was applied to S1, along the positive x direction, corresponding to a constant strain rate. A constant strain rate of 10^7 s^{-1} was chosen in the present work because Jian et al. [30] suggested using a critical strain rate to avoid nonphysical stress fluctuations. The shear deformation was performed for 2.5 million timesteps of 2 fs each. An NVT thermostat [31] implemented in LAMMPS was applied to regions B1 and B2 to maintain a constant temperature. No thermostat was used in regions A, C1, and C2.

Pure Mg and Mg–Ca alloys with Ca concentrations of 0.01 to 1 at.% at temperatures of 1 to 500 K were included in this study. In the Mg–Ca systems, Mg atoms were randomly substituted with Ca atoms with a probability equal to the atomic concentration. Stress–strain (S–S) curves were obtained from shear simulations, and the CRSS at 1 K was calculated from the peak stress value in the elastic deformation regime. The CRSS values for temperatures other than 1 K were taken as the average stress in the steady-state plastic deformation regime because the strength of local obstacles depended on the random distributions of the Ca atoms. To reduce the effect of the random substitution of Ca atoms on CRSS, three models with the same Ca concentration were constructed and used in the MD calculations, and the average value of the three data points was used in the analysis.

3. Results and discussion

3.1. Solute effect on S–S behavior

Fig. 2 shows the representative S–S curves of the Mg–Ca alloys with Ca solute concentrations of up to 1 at.% at a temperature of 300 K, on the basal plane. We observe an initial elastic deformation, which corresponds to an initial linear increase in the shear stress up to the peak stress value, followed by an abrupt drop with increasing shear strain, in all S–S curves. As the plastic deformation progresses, the flow stress fluctuates around an average value because of dislocation–phonon interactions. The CRSS exhibits a rapid increase with increasing solute concentration when the solute concentration is higher than 0.05 at.%. However, we do not observe a solution-strengthening effect when the solute concentration is lower than 0.05 at.%.

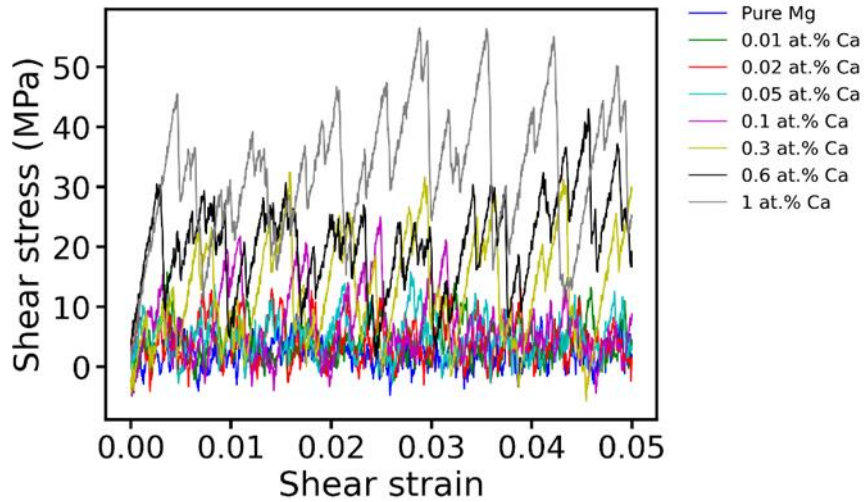


Fig. 2. Stress–strain curves obtained by applying shear strain to an Mg–Ca system containing an edge $\langle a \rangle$ dislocation, for various Ca solute concentrations at 300 K.

Fig. 3(a) shows the CRSS values extracted from the S–S curves, as a function of the solution concentration at finite temperatures. The change in the CRSS is small in the low-solute-concentration region ($c_{\text{Ca}} \leq 0.0005$) and becomes substantial in the higher-solute-concentration region ($c_{\text{Ca}} \geq 0.001$). Thus, we observe a solute-strengthening effect in the higher-solute-concentration region; however, no solute-strengthening effect is observed when the Ca concentration is lower than 0.0005. Our results are consistent with the experimental results observed for the Mg–Sn [24],

Mg–Al [21], and Mg–Zn [20] alloys. Because more solute atoms surround the dislocations in the higher-solute-concentration region, a higher stress is required to overcome the solute barriers, and solution strengthening can be observed. Fig. 3(b) shows the solute-strengthening scaling component, n , obtained by calculating the slopes of the various curves at various temperatures, presented in Fig. 3(a). When the solute concentration is ≤ 0.005 (0.05 at.%), the solute-strengthening scaling component decreases with increasing temperature because the thermal vibrations of the crystal atoms can facilitate basal dislocation in a manner that overcomes obstacles at lower stresses than that required at 0 K. However, when the concentration is ≥ 0.001 (0.1 at.%), the n value increases slightly with increasing temperature, but is close to the value of $1/2$ observed in other Mg alloys [20].

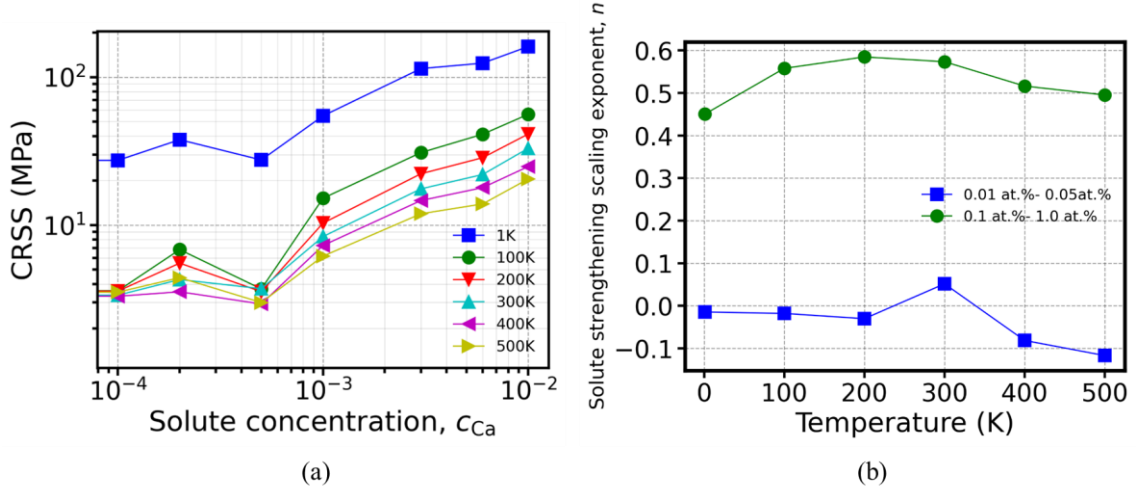


Fig. 3. (a) Variations in CRSS for edge $\langle a \rangle$ dislocations on the basal plane, as a function of the solution concentration c_{Ca} at temperatures ranging from 1 to 500 K. (b) Solute-strengthening scaling exponent n calculated from the slopes of the curves shown in Fig. 3(a), as a function of temperature.

Based on these results, the CRSS for the Mg–Ca alloys can be written as follows:

$$\tau(T, c) = \tau_0(c) + A(T)c^{\frac{1}{2}}, \quad (1)$$

where τ is the CRSS, τ_0 is the CRSS as a function of the solution concentration c as temperature $T \rightarrow 0$ K, and A is a temperature-dependent parameter. We replot the data points in Fig. 3(a) as functions of $c^{1/2}$ (Fig. 4). As shown in Fig. 4, the CRSS is not perfectly linearly dependent on $c^{1/2}$. If we use Eq. (1), we must also fit parameter A for

various temperatures. Therefore, we cannot use Eq. (1) to predict the CRSS readily and accurately.

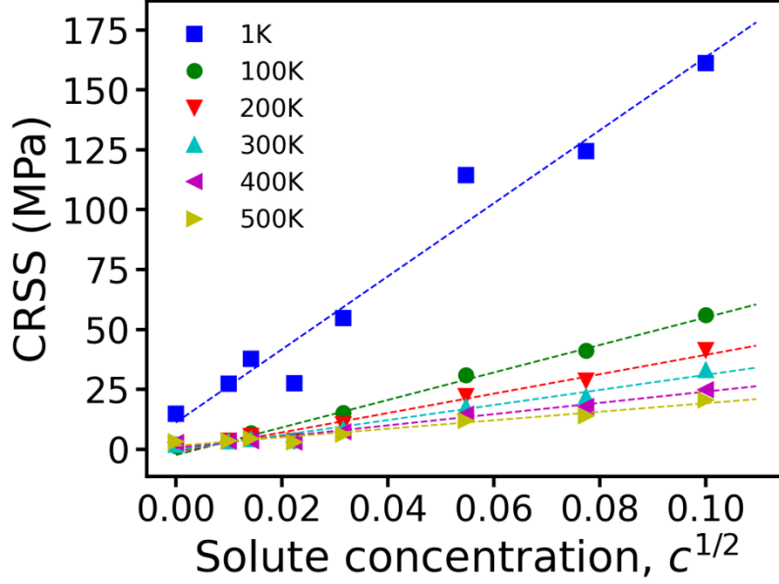


Fig. 4. Data points of Fig. 3 (a) replotted as functions of $c^{1/2}$.

3.2. Solute-strengthening model

Recently, Tehranchi et al. [32] developed an analytical formula for predicting the solute strengthening of basal slip in Mg alloys, including the effects of the solute elements, strain rate, and temperature. However, they claimed that there was a tendency for the theory to become less accurate with increasing concentration and reported the results at low concentrations and stresses (< 20 MPa) only, for several solutes (Al, Zn, Dy, and Y).

In this study, we propose the following relation for predicting the dependence of CRSS on the temperature and solute concentration by improving the Tehranchi et al. model as

$$\tau(c, T) = \tau_0 \exp\left(-\frac{1}{C_l} \left(\frac{k_B T}{\Delta E_b} \ln \frac{\dot{\epsilon}_0}{\dot{\epsilon}}\right)^n\right), \quad (2)$$

with

$$\tau_0 = kc^{\frac{1}{2}} + b, \quad (3)$$

and

$$\Delta E_b = c^{\frac{1}{3}} \Gamma^{\frac{1}{3}} \Delta \bar{E}_b. \quad (4)$$

Here C_l is a constant derived in [33], k_B is the Boltzmann constant, $\dot{\epsilon}_0$ is the reference strain rate, $\dot{\epsilon}$ is the experimental strain rate, k and b are the parameters obtained by fitting the CRSS at 1 K with the various Ca concentrations used in this work, Γ is the dislocation line tension used in [33], and $\Delta \bar{E}_b$ is the energy barrier calculated in [32]. In accordance with the relevant results of the solution-strengthening component [Fig. 3(b)], we chose $n = 0.05$ when $c \leq 0.0005$ (0.05 at.%) and $n = 0.5$ when $c \geq 0.001$ (0.1 at.%). Table 1 lists the values of the various parameters used in this study.

Table 1. Values of various parameters used in our solute-strengthening model.

C_l	$\dot{\epsilon}_0$ (s^{-1})	$\dot{\epsilon}$ (s^{-1})	k (MPa)	b (MPa)	Γ (eV/Å)	$\Delta \bar{E}_b$ (Å ^{1/3} eV ^{2/3})
0.55	10^4	2.3×10^{-4}	1524	11	0.4	3.956

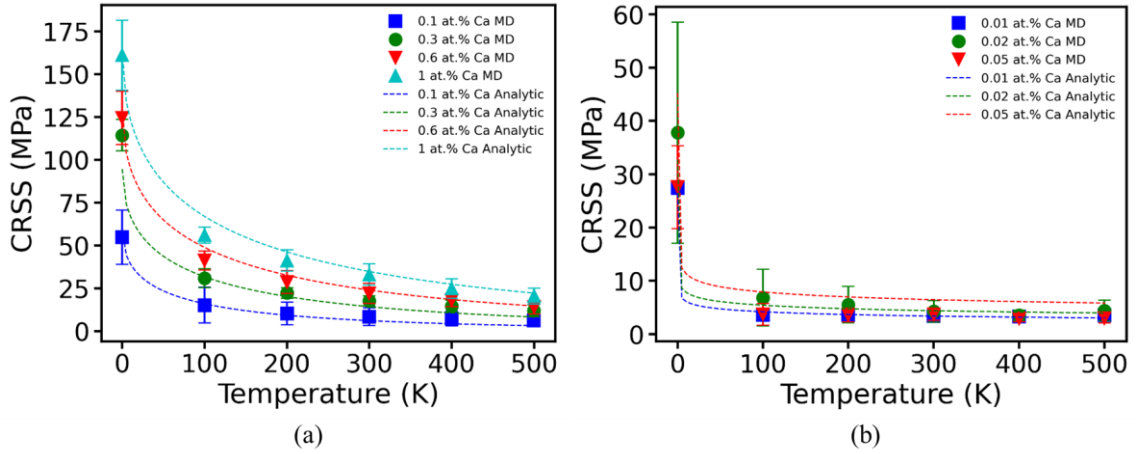


Fig. 5. CRSS for basal slip versus temperature for Mg–Ca alloys at concentrations (a) ≥ 0.1 at.% and (b) ≤ 0.05 at.%. The markers represent the MD simulation results. We plotted the dashed lines by applying our analytical solute-strengthening model. The error bars represent the standard deviations.

Fig. 5 compares the predicted values of the CRSS for the basal slip in Mg–Ca alloys with our simulation results. The predicted CRSS values are in excellent agreement with almost all our simulation results, including those at concentrations ≤ 0.05 at.% [Fig. 5(b)] and ≥ 0.1 at.% [Fig. 5(a)]. For the solute concentration of 1 wt. %, we overestimated the CRSS by several MPa; however, the CRSS was still accurate enough to be used as a prediction value.

3.3. Micropillar compression tests

Because we could not find available experimental values for the CRSS of single-crystalline Mg–Ca alloys from previous research for comparison, we performed micropillar compression tests to obtain the CRSS and thus validate our solute-strengthening model.

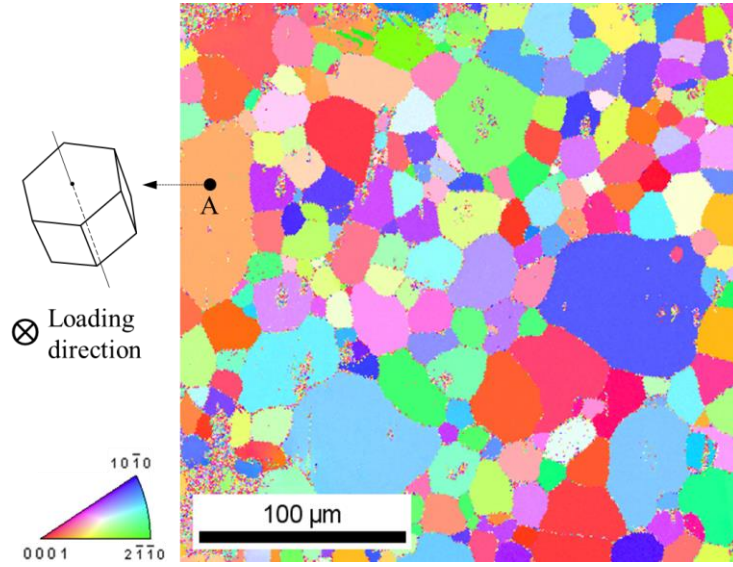


Fig. 6. Electron backscatter diffraction (EBSD) map indicating the orientations of the crystals (as given by the inverse pole figure) in the Mg–Ca sample used in the present work. We selected grain A (loading direction perpendicular to the image, forming an angle of $\sim 50^\circ$ with respect to $[0\ 0\ 0\ 1]$), to carve the micropillars.

We used Mg–0.3at.%Ca and Mg–0.6at.%Ca alloys in this work. We obtained the crystallographic orientations of the grains in the samples using a JSM-IT100 (JEOL Ltd.) equipped with a scanning electron microscope and an electron backscatter

diffraction (EBSD) detector. We selected grain A with specific orientations to favor the basal deformation modes (Fig. 6).

The micropillars were milled at the center of the selected grains using a focused ion beam JIB-4000 (JEOL Ltd.). We prepared the micropillars with a square cross section of approximately $5\text{ }\mu\text{m} \times 5\text{ }\mu\text{m}$ and an aspect ratio of 2:1 to 3:1. We confirmed that the size effects on the flow stress were minimal in Mg and Mg alloys of these dimensions through our pre-experimental tests; some previous studies have also reported similar results regarding size effects [13, 34].

We conducted micropillar compression tests using a nanoindenter G200 (KLA Corp.). We attached a diamond cylindrical flat punch of $20\text{ }\mu\text{m}$ diameter to the indenter tip to compress the micropillars. We performed all the tests at a constant strain rate of $5 \times 10^{-4}\text{ s}^{-1}$ under displacement control.

Fig. 7(a) and 7(b) show the nominal S–S curves of the micropillars of Mg–0.3at.%Ca and Mg–0.6at.%Ca, respectively. Gradual yielding of the micropillars was followed by a stage in which the deformation progressed at a constant stress. We calculated the CRSS values using Schmid’s law and used the yield stresses and Euler angles extracted from the experiments. Tables 2 and 3 present the CRSS values.

Table 2. CRSS on the basal plane of Mg–0.3at.%Ca pillars.

Sample	CRSS on the basal plane (MPa)
S1	16.8
S2	22.7
S3	19.8
S4	19.7
S5	8.7
S6	15.5

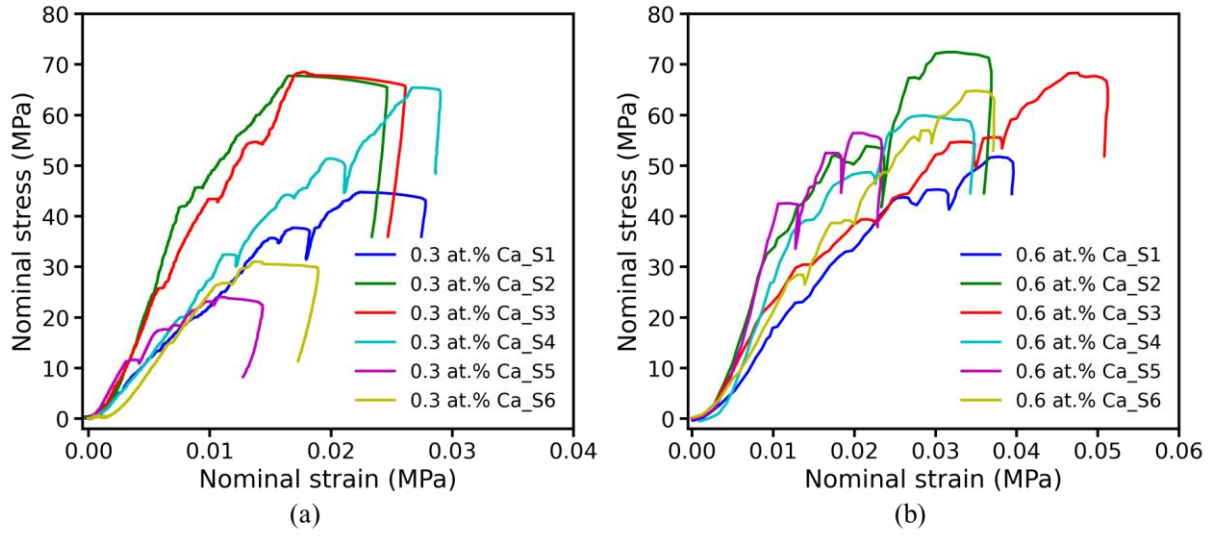


Fig. 7. Stress–strain curves of micropillar compression tests in (a) micropillars (S1–S6) of Mg–0.3at.%Ca alloys and (b) micropillars (S1–S6) of Mg–0.6at.% Ca alloys.

Table 3 CRSS on the basal plane of Mg–0.6at.%Ca pillars.

Sample	CRSS on the basal plane (MPa)
S1	21.7
S2	20.7
S3	26.1
S4	23.2
S5	20.8
S6	29.3

Using our solute-strengthening model, we compared the predicted and experimental values of CRSS for Mg–0.3at.%Ca and Mg–0.6at.% Ca alloys (Fig. 8). Our analytical model predicted the CRSS for both concentrations with high accuracy. Thus, by modifying the parameters used in the solute-strengthening model, we may be able to accurately assess the solute-strengthening effects of many other solute elements in binary Mg alloys.

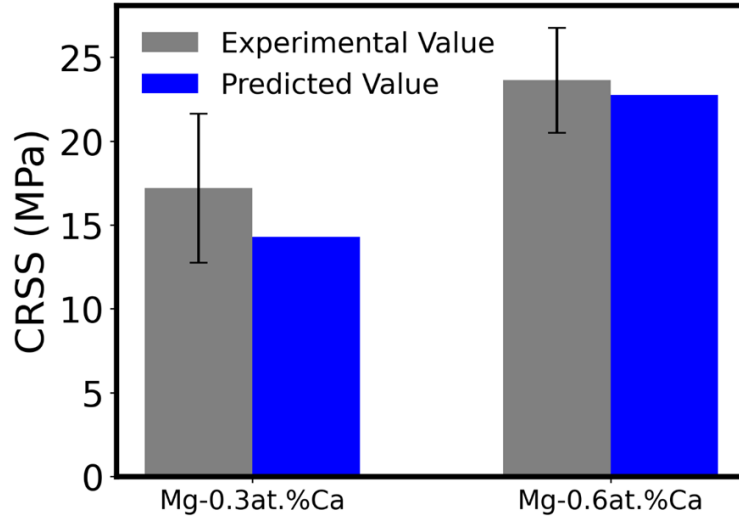


Fig. 8. Comparison of experimental CRSS and CRSS predicted by our solute-strengthening model for Mg-0.3at.%Ca and Mg-0.6at.%Ca alloys. Error bars represent the standard deviation.

4. Conclusions

We systematically studied solute strengthening in single-crystal Mg-Ca alloys at finite temperatures. When the concentration of the Ca solute was ≤ 0.05 at.%, the solute-strengthening component was < 0.1 , which indicated a low or no solute-strengthening effect. These results were consistent with those observed for Mg-Zn, Mg-Al, and Mg-Sn alloys. When the concentration of the Ca solute was ≥ 0.1 at.%, the solute-strengthening component was close to $1/2$, as predicted by the Butt-Feltham model [22], but this result depended on the temperature. We also proposed an analytical formula to predict the Mg-Ca alloy solute strengthening on the basal plane, which also considered the temperature dependence. The values of the CRSS predicted using the proposed formula agreed well with our simulation results, and we validated them with our experimental results.

Data availability

Data will be made available on request.

Acknowledgments

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