Title:

Equilibrium shape of isolated precipitates in the α -Mg phase

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Abstract

The habit plane of an isolated plate-shaped precipitate in an α -Mg matrix was calculated as a function of the stress-free transformation strain (i.e., the lattice mismatch between the precipitate and α -Mg matrix) using micromechanics. The results were categorized into 10 cases according to the habit-plane orientation, and the conditions for prismatic plate precipitation (i.e., $\{01\bar{1}0\}_\alpha$ or $\{2\bar{1}\bar{1}0\}_\alpha$ plates), which is assumed to be the most effective type of precipitation for dispersion strengthening for a given volume fraction and number density of a precipitate, were revealed. Furthermore, it was demonstrated that the equilibrium shape of precipitates (the plate- and rod-shaped precipitates often observed in Mg-based alloys) can be explained in terms of minimization of the strain energy associated with precipitation. The obtained results are believed to be essential for attempting precipitate shape control through the optimization of the lattice parameters of the precipitates and matrix phase.

Keywords: Mg-based alloys; precipitation hardening; misfit strain; morphological stability; micromechanics

1. Introduction

The age hardening of Mg-based alloys has attracted substantial attention as a method for enabling their use in various structural components. In age-hardened Mg-based alloys [1–17], precipitates, and Guinier–Preston (GP) zones with various morphologies, such as $[0001]_{\alpha}$ rods, $\langle 01\bar{1}0 \rangle_{\alpha}$ or $\langle 2\bar{1}\bar{1}0 \rangle_{\alpha}$ rods, $(0001)_{\alpha}$ plates (basal plates), and $\{01\bar{1}0\}_{\alpha}$ or $\{2\bar{1}\bar{1}0\}_{\alpha}$ plates (prismatic plates), have been observed experimentally in the hexagonal α -Mg phase. With respect to Orowan strengthening [18], plate-shaped precipitates that form on the prismatic planes ($\{01\bar{1}0\}_{\alpha}$ or $\{2\bar{1}\bar{1}0\}_{\alpha}$) of the α -Mg phase have been shown to be the most effective for dispersion strengthening when plastic deformation predominantly occurs via the motion of dislocations gliding on the $(0001)_{\alpha}$ slip plane of the α -Mg phase [19]. Although the effectiveness of a precipitate depends on its morphology (shape and orientation) for a given precipitate volume fraction and number density, a comprehensive understanding of the formation mechanism of plate- and rod-shaped precipitates in Mg-based alloys has not yet been achieved.

The equilibrium shape of a precipitate is determined by the interplay between the interface energy and strain energy [20]. Gao et al. [21] developed a phase-field model in which the interface energy was assumed to be isotropic and simulated the equilibrium shape of an isolated β_1 precipitate (intermediate phase) in a Mg–Y–Nd alloy. They revealed that the $(01\bar{1}0)_{\alpha}$ habit plane of a disk-shaped β_1 precipitate is completely determined by the minimization of the anisotropic strain energy. Liu et al. [22], meanwhile, simulated the effects of anisotropy in the interface energy and strain energy on the morphology of β' precipitates (intermediate phase) in Mg–Y and Mg–Gd alloys, and found that although the equilibrium shape of β' precipitates is influenced by both interface energy anisotropy and strain energy anisotropy, the shape variation of the β' precipitates is sensitive to the change in the lattice parameters of the precipitates and matrix phase, i.e., the change in the strain energy anisotropy.

First-principles calculations revealing the coherency strain effects on the prismatic habit plane morphology of metastable β'' -D0₁₉ precipitates in Mg alloys have also been reported [23]. These previous studies suggest that precise knowledge of the relationship between the conditions for stress-free transformation strain (i.e., the magnitude and anisotropy of the lattice mismatch between a precipitate and the α -Mg matrix) and the habit-plane orientations is essential for precipitate shape control. In fact, Zhang and Kelly [24,25] predicted the orientation relationships and habit planes of Mg₁₇Al₁₂ precipitates in a Mg–Al alloy and Mg₂₅Y₅ precipitates in a Mg–Y alloy using the edge-to-edge matching model and suggested that the lattice parameters of both the precipitates and matrix phase [5,6] strongly affect the habit plane orientations.

According to micromechanics [20,26], the strain energy of an isolated coherent inclusion within an infinite anisotropic matrix is dependent on the shape and orientation of the inclusion. The minimum strain energy at a given inclusion volume is attained if the inclusion is an infinite platelet of infinitesimal thickness whose habit-plane orientation is dependent on the stress-free transformation strain. Thus, whether plate-shaped precipitates on the $\{01\bar{1}0\}_\alpha$ or $\{2\bar{1}\bar{1}0\}_\alpha$ planes are formed depends on the magnitude and anisotropy of the stress-free transformation strain. In this study, therefore, we calculated the habit plane of a plate-shaped precipitate in the hexagonal α -Mg matrix phase as a function of the stress-free transformation strain using Khachaturyan and Shatalov's microelasticity theory [20]. The obtained results were then categorized according to the habit-plane orientations. The focus was on the conditions for prismatic plate precipitation that contributes to the strengthening of Mg-based alloys. Furthermore, using the calculated results, the mechanism of formation of both plate-shaped and rod-shaped precipitates in Mg-based alloys was explored in terms of the strain energy anisotropy.

2. Calculation method

In an elastically homogeneous system, the equation for the strain energy of an isolated coherent inclusion within an infinite anisotropic matrix is written as follows [20]:

$$E = \frac{1}{2} \int_{\mathbf{k}} B(\mathbf{n}) |s(\mathbf{k})| \frac{d\mathbf{k}}{(2\pi)^3}, \quad (1)$$

where $\mathbf{k}$ is the reciprocal-space vector, $s(\mathbf{k})$ is the Fourier transformation of the shape function of an arbitrary shaped coherent inclusion, and

$$B(\mathbf{n}) \equiv C_{ijkl} \varepsilon_{ij}^0 \varepsilon_{kl}^0 - n_i \sigma_{ij}^0 \Omega_{jl}(\mathbf{n}) \sigma_{lm}^0 n_m, \quad (2)$$

which is the function of the direction $\mathbf{n} = \mathbf{k}/|\mathbf{k}|$. Here C_{ijkl} is the elastic modulus tensor, ε_{ij}^0 is the arbitrary stress-free transformation strain, σ_{ij}^0 is defined as

$$\sigma_{ij}^0 \equiv C_{ijkl} \varepsilon_{kl}^0, \quad (3)$$

and $\Omega_{ij}(\mathbf{n})$ is the inverse tensor to

$$\Omega_{ij}^{-1}(\mathbf{n}) \equiv C_{ikjl} n_k n_l. \quad (4)$$

The strain energy given by Eq. (1) is minimized for a plate-like inclusion whose aspect ratio approaches zero and whose habit plane is normal to the vector $\mathbf{n} = \mathbf{n}_0$ corresponding to the minimum of the function $B(\mathbf{n})$; i.e., the determination of the habit-plane orientation ($\mathbf{n}_0$) of a precipitate is reduced to the minimization of $B(\mathbf{n})$ with respect to the vector $\mathbf{n}$. If a rearrangement of the crystal lattice from one orthorhombic phase to another is assumed, the stress-free transformation strain (the crystal lattice mismatch between the precipitate and

matrix phase) is given by

$$\varepsilon_{ij}^0 = \begin{pmatrix} \varepsilon_{11}^0 & 0 & 0 \\ 0 & \varepsilon_{22}^0 & 0 \\ 0 & 0 & \varepsilon_{33}^0 \end{pmatrix}, \quad (5)$$

where

$$\varepsilon_{11}^0 = \frac{a-a_0}{a_0}, \quad \varepsilon_{22}^0 = \frac{b-b_0}{b_0}, \quad \text{and} \quad \varepsilon_{33}^0 = \frac{c-c_0}{c_0}. \quad (6)$$

Here a , b , and c are the crystal lattice parameters of the precipitate, and a_0 , b_0 , and c_0 are the crystal lattice parameters of the matrix phase. The crystal lattice rearrangement accompanied by nonzero shear components of the stress-free transformation strain (ε_{ij}^0 , $i \neq j$) is the subject of a separate paper and will be reported elsewhere. The nonzero components of the elastic modulus tensor of an orthorhombic crystal are as follows:

$$\begin{aligned} C_{1111} &= C_{11}, \quad C_{2222} = C_{22}, \quad C_{3333} = C_{33}, \\ C_{1122} &= C_{12}, \quad C_{1133} = C_{13}, \quad C_{2233} = C_{23}, \\ C_{2323} &= C_{44}, \quad C_{3131} = C_{55}, \quad C_{1212} = C_{66}, \end{aligned} \quad (7)$$

where C_{ij} is the Voigt elastic constant. The substitution of the tensor ε_{ij}^0 from Eq. (5) into Eq. (2) gives

$$B(\mathbf{n}) = \bar{B} - \psi(\mathbf{n}), \quad (8)$$

where

$$\bar{B} \equiv C_{ijkl} \varepsilon_{ij}^0 \varepsilon_{kl}^0 = \varepsilon_{11}^0 \sigma_{11}^0 + \varepsilon_{22}^0 \sigma_{22}^0 + \varepsilon_{33}^0 \sigma_{33}^0, \quad (9)$$

$$\begin{aligned}
\sigma_{11}^0 &= C_{11}\varepsilon_{11}^0 + C_{12}\varepsilon_{22}^0 + C_{13}\varepsilon_{33}^0, \\
\sigma_{22}^0 &= C_{12}\varepsilon_{11}^0 + C_{22}\varepsilon_{22}^0 + C_{23}\varepsilon_{33}^0, \\
\sigma_{33}^0 &= C_{13}\varepsilon_{11}^0 + C_{23}\varepsilon_{22}^0 + C_{33}\varepsilon_{33}^0,
\end{aligned}$$

and

$$\begin{aligned}
\psi(\mathbf{n}) &\equiv \frac{A_1(\mathbf{n})+A_2(\mathbf{n})+A_3(\mathbf{n})+2\{A_4(\mathbf{n})+A_5(\mathbf{n})+A_6(\mathbf{n})\}}{D(\mathbf{n})}, \quad (10) \\
D(\mathbf{n}) &\equiv (C_{11}n_1^2 + C_{66}n_2^2 + C_{55}n_3^2)(C_{22}n_2^2 + C_{44}n_3^2 + C_{66}n_1^2)(C_{33}n_3^2 + C_{55}n_1^2 + C_{44}n_2^2) \\
&\quad + 2(C_{12} + C_{66})(C_{23} + C_{44})(C_{13} + C_{55})n_1^2n_2^2n_3^2 \\
&\quad - (C_{11}n_1^2 + C_{66}n_2^2 + C_{55}n_3^2)(C_{23} + C_{44})^2n_2^2n_3^2 \\
&\quad - (C_{22}n_2^2 + C_{44}n_3^2 + C_{66}n_1^2)(C_{13} + C_{55})^2n_3^2n_1^2 \\
&\quad - (C_{33}n_3^2 + C_{55}n_1^2 + C_{44}n_2^2)(C_{12} + C_{66})^2n_1^2n_2^2,
\end{aligned}$$

$$\begin{aligned}
A_1(\mathbf{n}) &\equiv n_1^2\{-(C_{23} + C_{44})^2n_2^2n_3^2 + (C_{55}n_1^2 + C_{44}n_2^2 + C_{33}n_3^2)(C_{66}n_1^2 + C_{22}n_2^2 + C_{44}n_3^2)\}(\sigma_{11}^0)^2, \\
A_2(\mathbf{n}) &\equiv n_2^2\{-(C_{13} + C_{55})^2n_3^2n_1^2 + (C_{66}n_2^2 + C_{55}n_3^2 + C_{11}n_1^2)(C_{44}n_2^2 + C_{33}n_3^2 + C_{55}n_1^2)\}(\sigma_{22}^0)^2, \\
A_3(\mathbf{n}) &\equiv n_3^2\{-(C_{12} + C_{66})^2n_1^2n_2^2 + (C_{44}n_3^2 + C_{66}n_1^2 + C_{22}n_2^2)(C_{55}n_3^2 + C_{11}n_1^2 + C_{66}n_2^2)\}(\sigma_{33}^0)^2, \\
A_4(\mathbf{n}) &\equiv n_1^2n_2^2\{(C_{23} + C_{44})(C_{13} + C_{55})n_3^2 - (C_{12} + C_{66})(C_{55}n_1^2 + C_{44}n_2^2 + C_{33}n_3^2)\sigma_{11}^0\sigma_{22}^0\}, \\
A_5(\mathbf{n}) &\equiv n_2^2n_3^2\{(C_{13} + C_{55})(C_{12} + C_{66})n_1^2 - (C_{23} + C_{44})(C_{66}n_2^2 + C_{55}n_3^2 + C_{11}n_1^2)\sigma_{22}^0\sigma_{33}^0\}, \\
A_6(\mathbf{n}) &\equiv n_3^2n_1^2\{(C_{12} + C_{66})(C_{23} + C_{44})n_2^2 - (C_{13} + C_{55})(C_{44}n_3^2 + C_{66}n_1^2 + C_{22}n_2^2)\sigma_{33}^0\sigma_{11}^0\}.
\end{aligned}$$

In Eq. (8), $\bar{B}$ is a constant; hence, $B(\mathbf{n})$ reaches its minimum when the function $\psi(\mathbf{n})$ has a maximum value. In a spherical coordinate system, the vector $\mathbf{n}$ is written as follows:

$$\mathbf{n} = (n_1, n_2, n_3) = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta), \quad (11)$$

where θ is the angle between the vector $\mathbf{n}$ and z -axis, and ϕ is the angle between the projection of the vector $\mathbf{n}$ on the x - y plane and x -axis (see Fig. 1). Consequently, by substituting Eq. (11) into Eq. (10), we can rewrite the function $\psi(\mathbf{n})$ as a function of θ and ϕ . The values of θ_0 and ϕ_0 at which the function $\psi(\theta, \phi)$ reaches its maximum determine

the vector $\mathbf{n}_0$ normal to the habit plane. The values of θ_0 and ϕ_0 are found by solving the following equations:

$$\frac{\partial \psi(\theta, \phi)}{\partial \theta} = 0, \quad \frac{\partial \psi(\theta, \phi)}{\partial \phi} = 0, \quad (12.a)$$

$$\frac{\partial^2 \psi(\theta, \phi)}{\partial \theta^2} < 0, \quad (12.b)$$

and

$$\left(\frac{\partial^2 \psi(\theta, \phi)}{\partial \theta \partial \phi} \right)^2 - \left(\frac{\partial^2 \psi(\theta, \phi)}{\partial \theta^2} \right) \left(\frac{\partial^2 \psi(\theta, \phi)}{\partial \phi^2} \right) < 0. \quad (12.c)$$

3. Results

The habit plane of an isolated plate-shaped inclusion in the α -Mg matrix was calculated. As shown in Fig. 1, the Cartesian coordinate axes x , y , and z in a hexagonal crystal were assumed to correspond to the $[2\bar{1}\bar{1}0]_\alpha$, $[01\bar{1}0]_\alpha$, and $[0001]_\alpha$ of the α -Mg matrix, respectively. The following elastic constants (in units of 10^{11} Pa) for the α -Mg phase were used in the analysis [27]: $C_{11} = C_{22} = 0.597$, $C_{33} = 0.617$, $C_{12} = 0.262$, $C_{13} = C_{23} = 0.217$, $C_{44} = C_{55} = 0.164$, and $C_{66} = (C_{11} - C_{12})/2$. Eqs. (12.a)–(12.c) were solved using the computational software Mathematica, whose visualization tools were used to prepare some of the figures presented in Section 3. The calculated results were categorized into 10 groups based on the habit-plane orientations. Among the 10 groups, plate-shaped inclusions on the prismatic planes of the α -Mg matrix were favorable in “Case 1” and “Case 2,” as shown below. The other eight cases (“Case 3” to “Case 10”) are summarized in the Appendix.

In “Case 1,” the habit-plane orientation of a plate-shaped inclusion is $\mathbf{n}_0 = (0, 1, 0)$ (a $[01\bar{1}0]_\alpha$ plate-shaped precipitate) when the stress-free transformation strain satisfies the following conditions:

$$\begin{cases} \left(\varepsilon_{22}^0 \leq \varepsilon_{11}^0 \text{ and } a_1^{(1)} < \varepsilon_{33}^0 < a_2^{(1)} \right) \\ \text{or} \\ \left(a_3^{(1)} < \varepsilon_{22}^0 \text{ and } a_4^{(1)} \leq \varepsilon_{33}^0 < a_1^{(1)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 < 0, \quad (13.a)$$

$$\begin{cases} \left(\varepsilon_{22}^0 < 0 \text{ and } a_5^{(1)} < \varepsilon_{33}^0 < 0 \right) \\ \text{or} \\ \left(\varepsilon_{22}^0 > 0 \text{ and } 0 < \varepsilon_{33}^0 < a_5^{(1)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 = 0, \quad (13.b)$$

and

$$\begin{cases} \left(\varepsilon_{22}^0 < a_3^{(1)} \text{ and } a_1^{(1)} < \varepsilon_{33}^0 \leq a_4^{(1)} \right) \\ \text{or} \\ \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 \text{ and } a_2^{(1)} < \varepsilon_{33}^0 < a_1^{(1)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 > 0. \quad (13.c)$$

Please see the Appendix for the $a_i^{(1)}$ values. In Fig. 2, the colored regions in the $\varepsilon_{11}^0 - \varepsilon_{22}^0 - \varepsilon_{33}^0$ space correspond to the conditions given by Eqs. (13.a)–(13.c). In “Case 2,” the habit-plane orientation of a plate-shaped inclusion is $\mathbf{n}_0 = (1, 0, 0)$ (a $(2\bar{1}\bar{1}0)_a$ plate-shaped precipitate) when the stress-free transformation strain satisfies

$$\begin{cases} \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 \leq 0 \text{ and } a_1^{(2)} < \varepsilon_{33}^0 < a_2^{(2)} \right) \\ \text{or} \\ \left(0 < \varepsilon_{22}^0 < a_3^{(2)} \text{ and } a_1^{(2)} < \varepsilon_{33}^0 < a_4^{(2)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 < 0, \quad (14.a)$$

and

$$\begin{cases} \left(a_3^{(2)} < \varepsilon_{22}^0 < 0 \text{ and } a_4^{(2)} \leq \varepsilon_{33}^0 < a_1^{(2)} \right) \\ \text{or} \\ \left(0 \leq \varepsilon_{22}^0 \leq \varepsilon_{11}^0 \text{ and } a_2^{(2)} < \varepsilon_{33}^0 < a_1^{(2)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 > 0 \quad (14.b)$$

(see the Appendix for the $a_i^{(2)}$ values). The conditions given by Eqs. (14.a) and (14.b) are shown in Fig. 3 as the colored regions in the $\varepsilon_{11}^0 - \varepsilon_{22}^0 - \varepsilon_{33}^0$ space. To verify the calculated

results, the case in which the stress-free transformation strain is given by $\varepsilon_{11}^0 = 0.014$, $\varepsilon_{22}^0 = 0.013$, and $\varepsilon_{33}^0 = 0.011$ was considered. This case satisfies the condition given by Eq. (14.b); hence, the function $B(\mathbf{n})$ given by Eq. (8) should have its global minimum when the vector $\mathbf{n}$ is parallel to the x -axis ($[2\bar{1}\bar{1}0]_a$ direction). Figure 4 (a) shows the orientation dependence of $B(\mathbf{n})$ normalized by $\bar{B}$. In the figure, the straight-line distance from the origin to the curvilinear surface of the white region corresponds to the magnitude of $B(\mathbf{n})/\bar{B}$. The x - z and x - y cross sections of Fig. 4 (a) are shown in Figs. 4 (b) and (c), respectively. The results in Figs. 4 (a)–(c) confirm that the global minimum of $B(\mathbf{n})$ appears when the habit-plane orientation $\mathbf{n}$ is parallel to the x -axis ($[2\bar{1}\bar{1}0]_a$ direction), whereas the maximum for $B(\mathbf{n})$ appears when $\mathbf{n}$ is parallel to the z -axis ($[0001]_a$ direction); i.e., the strain energy given by Eq. (1) is minimized with a plate-shaped inclusion whose habit plane is $(2\bar{1}\bar{1}0)_a$.

Liu et al. [22] calculated lattice parameters of β' -Mg₇Y, β' -Mg₇Gd, and Mg by a first-principles method. They subsequently calculated the stress-free transformation strain of β' -Mg₇Y as $\varepsilon_{11}^0 = 0.0299$, $\varepsilon_{22}^0 = 0.0183$, and $\varepsilon_{33}^0 = -0.00273$ and the stress-free transformation strain of β' -Mg₇Gd as $\varepsilon_{11}^0 = 0.0345$, $\varepsilon_{22}^0 = 0.0185$, and $\varepsilon_{33}^0 = -0.00270$ [22]. Both these cases satisfy the conditions established in Eq. (14.b); therefore, the habit plane of both β' -Mg₇Y and β' -Mg₇Gd is $(2\bar{1}\bar{1}0)_a$. This result is consistent with the result reported by Liu et al. [22] that the habit plane of β' that precipitates in both Mg–Y and Mg–Gd alloys is nearly parallel to $\{2\bar{1}\bar{1}0\}_a$ in terms of the strain energy anisotropy.

4. Discussion

4.1 Interplay between the interface energy and strain energy

With respect to strain energy, plate-shaped inclusions for which the habit plane is

dependent on the stress-free transformation strain (Eq. (5)) are energetically favorable. Notably, however, an interplay between the interface energy and strain energy exists [20–22, 28–31], and when there are large interface energies and a small crystal lattice mismatch, spherical inclusions should predominate. For an ellipsoidal inclusion ($x^2/a^2 + y^2/b^2 + z^2/c^2 = 1$) within an infinite anisotropic matrix, the strain energy is written as follows [26]:

$$E_{\text{strain}} = \frac{V_0}{2} C_{ijkl} \varepsilon_{kl}^0 (\varepsilon_{ij}^0 - S_{ijmn} \varepsilon_{mn}^0), \quad (15)$$

where V_0 is the volume of the inclusion, C_{ijkl} is the elastic modulus tensor, ε_{ij}^0 is the stress-free transformation strain, and S_{ijmn} is Eshelby's tensor. The ellipsoid is transformed into a unit sphere (S^2) by appropriate transformations of the variables, and S_{ijmn} is given by [26]

$$S_{ijmn} = \frac{abc}{4} C_{pqmn} \int_{S^2} \frac{\Omega_{pi}(\mathbf{n}) n_j n_q + \Omega_{pj}(\mathbf{n}) n_i n_q}{2} \frac{dS(\mathbf{n})}{(a^2 n_1^2 + b^2 n_2^2 + c^2 n_3^2)^{3/2}}, \quad (16)$$

where $\Omega_{ij}(\mathbf{n})$ is the inverse tensor to Eq. (4), and $dS(\mathbf{n})$ is the surface element on the unit sphere S^2 in the $\mathbf{k}$ -space. When a spheroidal inclusion is assumed ($a = b$, $p = c/a$), the sum of the strain energy and interface energy is given as follows:

$$\begin{aligned} E_{\text{total}}(p) &\equiv E_{\text{strain}}(p) + E_{\text{interface}}(p) \\ &= \frac{V_0}{2} C_{ijkl} \varepsilon_{kl}^0 (\varepsilon_{ij}^0 - S_{ijmn}(p) \varepsilon_{mn}^0) + A(p) \gamma, \end{aligned} \quad (17)$$

where $A(p)$ is the interface area and γ is the interface energy (in units of J m^{-2}). Notably, the interface energy anisotropy is ignored here, and its effect on the precipitate shape has been simulated by Liu et al. [22]. The interface area $A(p)$ is given by:

$$A(p) = \pi r_0^2 p^{-2/3} [2 + F(p)], \quad (18)$$

$$F(p) = \frac{2p^2}{\sqrt{1-p^2}} \ln \left(\frac{1+\sqrt{1-p^2}}{p} \right) \quad \text{if } p < 1,$$

$$F(p) = 2 \quad \text{if } p = 1,$$

$$F(p) = \frac{2p^2}{\sqrt{p^2-1}} \tan^{-1} \sqrt{p^2-1} \quad \text{if } p > 1,$$

where r_0 is the radius of a sphere with volume V_0 ($V_0 = 4\pi r_0^3/3$). In the following sections, γ and r_0 are assumed to be $\gamma = 0.1 \text{ J m}^{-2}$ and $r_0 = 50 \text{ nm}$ ($V_0 \sim 5.2 \times 10^5 \text{ nm}^3$), and the mechanisms for the formation of plate- and rod-shaped precipitates are discussed. **Because of the lack of experimental data, arbitrary stress-free transformation strains of precipitates are assumed in the calculations. However, even if another stress-free transformation strain of precipitates is assumed, the fundamental considerations presented in each of the following sections are not influenced as long as the precipitates prefer the same habit plane in terms of the strain energy anisotropy.**

4.2 Rod-shaped precipitate along the $[0001]_a$ direction

The stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.01$, $\varepsilon_{22}^0 = 0.01$, and $\varepsilon_{33}^0 = 0.002$ as an example. This condition is categorized as a “Case 1” condition (see Section 3), and the habit plane is $(01\bar{1}0)_a$. However, when $\varepsilon_{11}^0 = \varepsilon_{22}^0$, arbitrary plate-shaped inclusions with habit planes perpendicular to the $(0001)_a$ plane have a strain energy of the same magnitude. The zone axis of these habit planes is along the $[0001]_a$ direction, as schematically shown in Fig. 5. Figure 6 presents the total energy E_{total} (i.e., the sum of the strain and interface energies) given by Eq. (17) for a spheroidal inclusion as a function of the aspect ratio of the spheroid p . Here, the total energy of the spheroidal inclusion is normalized

by the total energy of the spherical inclusion with the same volume. In Fig. 6, three different cases are shown in which the rotation axis of the spheroid is parallel to the $[2\bar{1}\bar{1}0]_\alpha$, $[01\bar{1}0]_\alpha$, or $[0001]_\alpha$ direction. As evident in Fig. 6, the plates perpendicular to the $(0001)_\alpha$ plane (i.e., the $(01\bar{1}0)_\alpha$ and $(2\bar{1}\bar{1}0)_\alpha$ plates) are energetically more favorable than the $(0001)_\alpha$ basal plate. However, the most stable precipitate shape is the $[0001]_\alpha$ rod, which has the lowest total energy. Notably, the $[0001]_\alpha$ direction coincides with the zone-axis direction of the plate-shaped inclusions that have the lowest strain energy (see Fig. 5). As an example of a rod-shaped precipitate along the $[0001]_\alpha$ direction, the MgZn_2 (β_1') phase has been reported to grow as an $[0001]_\alpha$ rod because the lattice mismatch between the α -Mg and MgZn_2 phases along the $[0001]_\alpha$ direction (ε_{33}^0) is smaller than that along other directions (ε_{11}^0 and ε_{22}^0) [13,15]. This result is qualitatively consistent with our calculated results, which indicate that the $[0001]_\alpha$ rod is the most energetically favored shape when the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.01$, $\varepsilon_{22}^0 = 0.01$, and $\varepsilon_{33}^0 = 0.002$.

4.3 Plate-shaped precipitates on the $(0001)_\alpha$ basal plane

In this case, the stress-free transformation strain was assumed to be $\varepsilon_{11}^0 = 0.0007$, $\varepsilon_{22}^0 = 0.0007$, and $\varepsilon_{33}^0 = 0.002$ as an example. This condition is categorized as a “Case 10” condition (see Appendix), and the habit plane is $(0001)_\alpha$. Figure 7 shows the normalized total energy of a spheroidal inclusion as a function of the aspect ratio of the spheroid. The results in Fig. 7 indicate that the $(0001)_\alpha$ basal plate is the most energetically stable shape, although the contribution of the strain energy is relatively small; hence, the stable shape is close to spherical (note the scale of the vertical and horizontal axes in Fig. 7). In a Mg–Sn–Zn alloy [15], for example, the Mg_2Sn phase has been reported to heterogeneously nucleate at the tip of the MgZn_2 (β_1') rods along the $[0001]_\alpha$ direction, and the shape of the MgZn_2 phase has been reported to change from an $[0001]_\alpha$ rod to an $(0001)_\alpha$ disc during growth of the

Mg₂Sn phase. The authors assumed that the change in shape of the MgZn₂ phase was attributed to the change in the stress field around the MgZn₂ phase as the Mg₂Sn phase grew [15]. As shown in Figs. 6 and 7, if the stress field on the (0001)_α basal plane is largely relaxed as the Mg₂Sn phase grows and the effective stress-free transformation strain changes as

$$\begin{pmatrix} 0.01 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 0.002 \end{pmatrix} \Rightarrow \begin{pmatrix} 0.0007 & 0 & 0 \\ 0 & 0.0007 & 0 \\ 0 & 0 & 0.002 \end{pmatrix}, \quad (19)$$

the change in the shape of the MgZn₂ phase from an [0001]_α rod to an (0001)_α disc may presumably occur to reduce the strain energy associated with the precipitation of the MgZn₂ phase.

4.4 Rod-shaped precipitates along the $\langle 2\bar{1}\bar{1}0 \rangle_\alpha$ and $\langle 01\bar{1}0 \rangle_\alpha$ directions

Here, the stress-free transformation strain was assumed to be $\varepsilon_{11}^0 = 0.01$, $\varepsilon_{22}^0 = 0.005$, and $\varepsilon_{33}^0 = 0.009$ as an example. This condition is categorized as a “Case 5” condition (see Appendix), and the habit-plane orientations of a plate-shaped inclusion are $\mathbf{n}_0 = (0.893, 0, \pm 0.449)$; two habit planes are perpendicular to the $(01\bar{1}0)_\alpha$ plane, and the zone axis of the two habit planes is along the $[01\bar{1}0]_\alpha$ direction, as schematically shown by the dashed line in Fig. 8. Hence the $[01\bar{1}0]_\alpha$ rod is the most energetically stable shape, which can be deduced from the mechanism of formation of the $[0001]_\alpha$ rod-shaped precipitates discussed in Section 4.2. The mechanism of formation of $[2\bar{1}\bar{1}0]_\alpha$ rod-shaped precipitates can be explained with the same reasoning. For example, when the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.005$, $\varepsilon_{22}^0 = 0.01$, and $\varepsilon_{33}^0 = 0.009$ (categorized as a “Case 3” condition in the Appendix), there are two habit-plane orientations

for a plate-shaped inclusion, $\mathbf{n}_0 = (0, 0.893, \pm 0.449)$. Hence, the most favorable shape is a rod along the $[2\bar{1}\bar{1}0]_\alpha$ direction, which coincides with the zone-axis direction of the two habit planes. Rod-shaped precipitates along the $\langle 2\bar{1}\bar{1}0 \rangle_\alpha$ and $\langle 01\bar{1}0 \rangle_\alpha$ directions in alloy systems such as Mg–Bi–Zn [13], Mg–Ca–Zn [14], and Mg–Sn–Zn [15] have been reported. In the future, clarification of the orientation relationships between the precipitates and α -Mg phase may lead to the presumption of the stress-free transformation strain and the verification of the mechanism of formation of the $\langle 2\bar{1}\bar{1}0 \rangle_\alpha$ and $\langle 01\bar{1}0 \rangle_\alpha$ rod-shaped precipitates discussed here.

4.5 Plate-shaped precipitates on the $\{2\bar{1}\bar{1}0\}_\alpha$ and $\{01\bar{1}0\}_\alpha$ prismatic planes

For this calculation, the stress-free transformation strain was assumed to be $\varepsilon_{11}^0 = 0.004$, $\varepsilon_{22}^0 = 0.008$, and $\varepsilon_{33}^0 = 0.003$ as an example. This condition is categorized as a “Case 1” condition (see Section 3), and the habit plane is $(01\bar{1}0)_\alpha$. Figure 9 (a) shows the normalized total energy of a spheroidal inclusion as a function of the aspect ratio of the spheroid. As shown in Fig. 9 (a), the $(01\bar{1}0)_\alpha$ prismatic plate is the most energetically stable shape. Figure 9 (b) shows the calculated results when the size of the coherent inclusion is increased from $r_0 = 50$ nm to 500 nm. Although the curve geometries in Fig. 9 (b) differ from those in Fig. 9 (a), the most stable shape is the $(01\bar{1}0)_\alpha$ plate, regardless of the inclusion size. Thus, the possibility for the formation of $\{01\bar{1}0\}_\alpha$ prismatic-plate precipitates is solely determined by the condition of the stress-free transformation strain if the interface energy anisotropy is not considered. This condition is also true for plate-shaped precipitates on the $\{2\bar{1}\bar{1}0\}_\alpha$ prismatic planes; i.e., if the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.008$, $\varepsilon_{22}^0 = 0.004$, and $\varepsilon_{33}^0 = 0.003$ (categorized as a “Case 2” condition in Section 3), the most stable shape for the precipitate is a $(2\bar{1}\bar{1}0)_\alpha$ prismatic plate.

However, an interplay occurs between the interface energy and strain energy. Thus,

even if the stress-free transformation strain satisfies the conditions for prismatic plate precipitation, the precipitate shape is nearly spherical, and the aspect ratio is high ($c/a \sim 1$) when the contribution of the interface energy is larger than that of the strain energy. On the other hand, if the contribution of the strain energy is sufficiently large (see Fig. 9 (b) as an example), plate-shaped precipitates with a low aspect ratio ($c/a \ll 1$) can be formed during aging heat treatment, which appears to be the reason why prismatic plates with a low aspect ratio ($c/a \sim 0.04$) precipitated in a Mg–Ca–In alloy [16,17], and prismatic-plate precipitates with a high aspect ratio were observed in a Mg–Bi–Zn alloy [13].

The interface energy anisotropy, which is not covered in this study, also has a significant effect on the equilibrium shape of precipitates. Liu et al. [22] revealed that the nearly equiaxed shape of β' -Mg₇Y precipitates that have been observed experimentally is the result of competition between the anisotropic interface energy and the anisotropic strain energy [22]. Therefore, the anisotropies of the interface and strain energies actually influence the shape of the precipitates. However, Liu et al. [22] also revealed that the shape of precipitates is more sensitive to variations of the lattice parameters than to variation of interface energy anisotropy. In other words, control of the lattice parameters of the precipitates and those of the matrix phase can increase the strain energy anisotropy; hence, it effectively enables control of the precipitate shape, including the habit plane orientation and aspect ratio [22,25]. Therefore, it is assumed that the results obtained in this study can point the path toward an efficient alloy design; if the lattice parameters of the precipitates and matrix phase are obtained experimentally or using first-principles calculations [23], it is possible to predict the equilibrium shape of the precipitates in terms of the strain energy anisotropy. Having this capability will accelerate the exploration of rare-earth-free Mg-based alloys strengthened by prismatic plate precipitates.

5. Conclusions

The strain energy of an isolated plate-shaped inclusion in the α -Mg matrix is dependent on the conditions for stress-free transformation strain (i.e., the magnitude and anisotropy of the lattice mismatch between the precipitates and α -Mg matrix). Strain energy calculations based on micromechanics revealed that the habit-plane orientations of plate-shaped precipitates can be categorized into 10 groups. The calculated results suggested that the equilibrium shape of precipitates (experimentally observed plate- and rod-shaped precipitates) can be explained in terms of the strain energy minimization. In two of these cases, plate-shaped precipitates on prismatic planes ($\{01\bar{1}0\}_\alpha$ and $\{2\bar{1}\bar{1}0\}_\alpha$) are the most energetically favorable. This result suggests that prismatic plate precipitation can be realized if the lattice mismatch between the precipitates and α -Mg phase is appropriately controlled. Furthermore, by assuming a spheroidal precipitate and considering the total energy (the sum of the isotropic interface and anisotropic strain energies), we showed that the aspect ratio of a plate- or rod-shaped precipitate of a given size can be predicted. When the contribution of the strain energy is sufficiently larger than that of the interface energy, plate-shaped precipitates with a low aspect ratio ($c/a \ll 1$) or rod-shaped precipitates with a high aspect ratio ($c/a \gg 1$) are formed during aging heat treatment. This result also suggests that optimization of the lattice mismatch is necessary for controlling the shape of precipitates that affect the strength of Mg-based alloys.

Notably, in the above-mentioned results, the categorization of the habit-plane orientations of plate-shaped precipitates into 10 groups is assumed to be essential for attempting precipitate shape control and will accelerate the exploration of rare-earth-free Mg-based alloys strengthened by prismatic plate precipitates.

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Appendix

The eight additional cases (“Case 3” through “Case 10”) for which the habit plane of a plate-shaped inclusion is a plane other than one of the prismatic planes of the α -Mg matrix are described here. The habit-plane orientation $\mathbf{n}_0$ is shown in the Cartesian coordinate system, as defined in Fig. 1.

“Case 3”

$$\mathbf{n}_0 = \left(0, \quad \frac{1}{2} \sqrt{\frac{A_2^{(3)}}{A_1^{(3)}}}, \quad \pm \frac{1}{2} \sqrt{\frac{A_3^{(3)}}{A_1^{(3)}}} \right)$$

when the stress-free transformation strain satisfies the following:

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 \leq \varepsilon_{11}^0 \text{ and } a_1^{(3)} < \varepsilon_{33}^0 < a_2^{(3)} \right) \\ \text{or} \\ \left(a_3^{(3)} < \varepsilon_{22}^0 \leq a_4^{(3)} \text{ and } a_5^{(3)} \leq \varepsilon_{33}^0 < a_1^{(3)} \right) \\ \text{or} \\ \left(a_4^{(3)} < \varepsilon_{22}^0 \text{ and } a_2^{(3)} < \varepsilon_{33}^0 < a_1^{(3)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.1.a})$$

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 < 0 \text{ and } a_6^{(3)} < \varepsilon_{33}^0 < a_7^{(3)} \right) \\ \text{or} \\ \left(0 < \varepsilon_{22}^0 \text{ and } a_7^{(3)} < \varepsilon_{33}^0 < a_6^{(3)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 = 0, \quad (\text{A.1.b})$$

and

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 < a_4^{(3)} \text{ and } a_1^{(3)} < \varepsilon_{33}^0 < a_2^{(3)} \right) \\ \text{or} \\ \left(a_4^{(3)} \leq \varepsilon_{22}^0 < a_3^{(3)} \text{ and } a_1^{(3)} < \varepsilon_{33}^0 \leq a_5^{(3)} \right) \\ \text{or} \\ \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 \text{ and } a_2^{(3)} < \varepsilon_{33}^0 < a_1^{(3)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.1.c})$$

“Case 4”

$$\mathbf{n}_0 = \left(0, \sqrt{\frac{A_2^{(4)}}{2A_1^{(4)}}}, \pm \sqrt{\frac{A_3^{(4)}}{2A_1^{(4)}}} \right)$$

when the stress-free transformation strain satisfies the following:

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 \leq \varepsilon_{11}^0 \text{ and } a_1^{(4)} < \varepsilon_{33}^0 \right) \\ \text{or} \\ \left(a_2^{(4)} < \varepsilon_{22}^0 \text{ and } \varepsilon_{33}^0 \leq a_3^{(4)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.2.a})$$

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 < 0 \text{ and } 0 < \varepsilon_{33}^0 \right) \\ \text{or} \\ \left(0 < \varepsilon_{22}^0 \text{ and } \varepsilon_{33}^0 < 0 \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 = 0, \quad (\text{A.2.b})$$

and

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 < a_2^{(4)} \text{ and } a_3^{(4)} \leq \varepsilon_{33}^0 \right) \\ \text{or} \\ \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 \text{ and } \varepsilon_{33}^0 < a_1^{(4)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.2.c})$$

“Case 5”

$$\mathbf{n}_0 = \left(\frac{1}{2} \sqrt{\frac{A_2^{(5)}}{A_1^{(5)}}}, 0, \pm \frac{1}{2} \sqrt{\frac{A_3^{(5)}}{A_1^{(5)}}} \right)$$

when the stress-free transformation strain satisfies the following:

$$\begin{cases} \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 \leq a_1^{(5)} \text{ and } a_2^{(5)} < \varepsilon_{33}^0 < a_3^{(5)} \right) \\ \text{or} \\ \left(a_1^{(5)} < \varepsilon_{22}^0 < a_4^{(5)} \text{ and } a_2^{(5)} < \varepsilon_{33}^0 \leq a_5^{(5)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.3.a})$$

and

$$\begin{cases} \left(a_4^{(5)} < \varepsilon_{22}^0 \leq a_1^{(5)} \text{ and } a_5^{(5)} \leq \varepsilon_{33}^0 < a_2^{(5)} \right) \\ \text{or} \\ \left(a_1^{(5)} < \varepsilon_{22}^0 \leq \varepsilon_{11}^0 \text{ and } a_3^{(5)} < \varepsilon_{33}^0 < a_2^{(5)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.3.b})$$

“Case 6”

$$\mathbf{n}_0 = \left(\sqrt{\frac{A_2^{(6)}}{2A_1^{(6)}}}, \quad 0, \quad \pm \sqrt{\frac{A_3^{(6)}}{2A_1^{(6)}}} \right)$$

when the stress-free transformation strain satisfies the following:

$$\begin{cases} \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 \leq 0 \text{ and } a_1^{(6)} < \varepsilon_{33}^0 \right) \\ \text{or} \\ \left(0 < \varepsilon_{22}^0 < a_2^{(6)} \text{ and } a_3^{(6)} \leq \varepsilon_{33}^0 \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.3.a})$$

and

$$\begin{cases} \left(a_2^{(6)} < \varepsilon_{22}^0 < 0 \text{ and } \varepsilon_{33}^0 \leq a_3^{(6)} \right) \\ \text{or} \\ \left(0 \leq \varepsilon_{22}^0 \leq \varepsilon_{11}^0 \text{ and } \varepsilon_{33}^0 < a_1^{(6)} \right) \end{cases} \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.3.b})$$

“Case 7”

$$\mathbf{n}_0 = \left(\sqrt{\frac{A_2^{(7)}}{A_1^{(7)}}}, \quad \pm \sqrt{\frac{A_3^{(7)}}{A_1^{(7)}}}, \quad 0 \right)$$

when the stress-free transformation strain satisfies the following:

$$\left\{ \begin{array}{l} \left(0 < \varepsilon_{22}^0 \leq a_1^{(7)} \text{ and } a_2^{(7)} \leq \varepsilon_{33}^0 < a_3^{(7)} \right) \\ \text{or} \\ \left(a_1^{(7)} < \varepsilon_{22}^0 \leq a_4^{(7)} \text{ and } a_5^{(7)} < \varepsilon_{33}^0 < a_3^{(7)} \right) \\ \text{or} \\ \left(a_4^{(7)} < \varepsilon_{22}^0 \text{ and } a_5^{(7)} < \varepsilon_{33}^0 \leq a_2^{(7)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.4.a})$$

and

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 < a_4^{(7)} \text{ and } a_2^{(7)} \leq \varepsilon_{33}^0 < a_5^{(7)} \right) \\ \text{or} \\ \left(a_4^{(7)} \leq \varepsilon_{22}^0 \leq a_1^{(7)} \text{ and } a_3^{(7)} < \varepsilon_{33}^0 < a_5^{(7)} \right) \\ \text{or} \\ \left(a_1^{(7)} < \varepsilon_{22}^0 < 0 \text{ and } a_3^{(7)} < \varepsilon_{33}^0 \leq a_2^{(7)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.4.b})$$

“Case 8”

$$\mathbf{n}_0 = \left(\sqrt{\frac{1}{7} \left(-328 + \frac{335A_3^{(8)}}{A_1^{(8)}} \right) \left(\frac{A_4^{(8)}}{A_2^{(8)}} \right)}, \quad \sqrt{\frac{5}{7} \left(-328 + \frac{335A_3^{(8)}}{A_1^{(8)}} \right) \left(\frac{A_5^{(8)}}{A_2^{(8)}} \right)}, \quad \pm \sqrt{\frac{335}{7} \left(1 - \frac{A_3^{(8)}}{A_1^{(8)}} \right)} \right),$$

and

$$\mathbf{n}_0 = \left(\pm \sqrt{\frac{1}{7} \left(-328 + \frac{335A_3^{(8)}}{A_1^{(8)}} \right) \left(\frac{A_4^{(8)}}{A_2^{(8)}} \right)}, \quad \mp \sqrt{\frac{5}{7} \left(-328 + \frac{335A_3^{(8)}}{A_1^{(8)}} \right) \left(\frac{A_5^{(8)}}{A_2^{(8)}} \right)}, \quad \sqrt{\frac{335}{7} \left(1 - \frac{A_3^{(8)}}{A_1^{(8)}} \right)} \right)$$

when the stress-free transformation strain satisfies the following:

$$\left\{ \begin{array}{l} \left(0 < \varepsilon_{22}^0 < a_1^{(8)} \text{ and } a_2^{(8)} < \varepsilon_{33}^0 \leq a_3^{(8)} \right) \\ \text{or} \\ \left(a_1^{(8)} < \varepsilon_{22}^0 < a_4^{(8)} \text{ and } a_2^{(8)} < \varepsilon_{33}^0 \leq a_5^{(8)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.5.a})$$

and

$$\left\{ \begin{array}{l} \left(a_4^{(8)} < \varepsilon_{22}^0 < a_1^{(8)} \text{ and } a_5^{(8)} \leq \varepsilon_{33}^0 < a_2^{(8)} \right) \\ \text{or} \\ \left(a_1^{(8)} \leq \varepsilon_{22}^0 < 0 \text{ and } a_3^{(8)} \leq \varepsilon_{33}^0 < a_2^{(8)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.5.b})$$

“Case 9”

$$\mathbf{n}_0 = \left(\sqrt{\frac{5}{7} \left(-328 + \frac{335A_3^{(9)}}{A_1^{(9)}} \right) \left(\frac{A_4^{(9)}}{A_2^{(9)}} \right)}, \quad \sqrt{\frac{1}{7} \left(-328 + \frac{335A_3^{(9)}}{A_1^{(9)}} \right) \left(\frac{A_5^{(9)}}{A_2^{(9)}} \right)}, \quad \pm \sqrt{\frac{335}{7} \left(1 - \frac{A_3^{(9)}}{A_1^{(9)}} \right)} \right),$$

and

$$\mathbf{n}_0 = \left(\pm \sqrt{\frac{5}{7} \left(-328 + \frac{335A_3^{(9)}}{A_1^{(9)}} \right) \left(\frac{A_4^{(9)}}{A_2^{(9)}} \right)}, \quad \mp \sqrt{\frac{1}{7} \left(-328 + \frac{335A_3^{(9)}}{A_1^{(9)}} \right) \left(\frac{A_5^{(9)}}{A_2^{(9)}} \right)}, \quad \sqrt{\frac{335}{7} \left(1 - \frac{A_3^{(9)}}{A_1^{(9)}} \right)} \right)$$

when the stress-free transformation strain satisfies the following:

$$\left\{ \begin{array}{l} \left(a_1^{(9)} < \varepsilon_{22}^0 \leq a_2^{(9)} \text{ and } a_3^{(9)} \leq \varepsilon_{33}^0 < a_4^{(9)} \right) \\ \text{or} \\ \left(a_2^{(9)} < \varepsilon_{22}^0 \text{ and } a_5^{(9)} \leq \varepsilon_{33}^0 < a_4^{(9)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.6.a})$$

and

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 \leq a_2^{(9)} \text{ and } a_4^{(9)} < \varepsilon_{33}^0 \leq a_5^{(9)} \right) \\ \text{or} \\ \left(a_2^{(9)} < \varepsilon_{22}^0 < a_1^{(9)} \text{ and } a_4^{(9)} < \varepsilon_{33}^0 \leq a_3^{(9)} \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.6.b})$$

“Case 10”

$$\mathbf{n}_0 = (0, \quad 0, \quad 1)$$

when the stress-free transformation strain satisfies the following:

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 \leq \varepsilon_{11}^0 \text{ and } \varepsilon_{33}^0 < a_1^{(10)} \right) \\ \text{or} \\ \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 < a_2^{(10)} \text{ and } \varepsilon_{33}^0 < a_3^{(10)} \right) \\ \text{or} \\ \left(a_4^{(10)} < \varepsilon_{22}^0 \text{ and } a_1^{(10)} < \varepsilon_{33}^0 \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 < 0, \quad (\text{A.7.a})$$

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 < 0 \text{ and } \varepsilon_{33}^0 < a_5^{(10)} \right) \\ \text{or} \\ \left(0 < \varepsilon_{22}^0 \text{ and } a_5^{(10)} < \varepsilon_{33}^0 \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 = 0, \quad (\text{A.7.b})$$

and

$$\left\{ \begin{array}{l} \left(\varepsilon_{22}^0 < a_4^{(10)} \text{ and } \varepsilon_{33}^0 < a_1^{(10)} \right) \\ \text{or} \\ \left(a_2^{(10)} < \varepsilon_{22}^0 < \varepsilon_{11}^0 \text{ and } a_3^{(10)} < \varepsilon_{33}^0 \right) \\ \text{or} \\ \left(\varepsilon_{11}^0 \leq \varepsilon_{22}^0 \text{ and } a_1^{(10)} < \varepsilon_{33}^0 \right) \end{array} \right. \quad \text{if } \varepsilon_{11}^0 > 0. \quad (\text{A.7.c})$$

All of the parameters in the above equations are summarized as follows:

$$a_1^{(1)} = \alpha_3 \varepsilon_{11}^0 + \alpha_4 \varepsilon_{22}^0, \quad a_2^{(1)} = \alpha_{10} \varepsilon_{11}^0, \quad a_3^{(1)} = \alpha_6 \varepsilon_{11}^0,$$

$$a_4^{(1)} = \alpha_{14} \varepsilon_{11}^0, \quad a_5^{(1)} = \alpha_{15} \varepsilon_{22}^0,$$

$$a_1^{(2)} = \alpha_4 \varepsilon_{11}^0 + \alpha_3 \varepsilon_{22}^0, \quad a_2^{(2)} = \alpha_{10} \varepsilon_{22}^0, \quad a_3^{(2)} = \alpha_7 \varepsilon_{11}^0, \quad a_4^{(2)} = \alpha_{14} \varepsilon_{22}^0,$$

$$a_1^{(3)} = \alpha_1 \varepsilon_{11}^0 + \alpha_2 \varepsilon_{22}^0, \quad a_2^{(3)} = \alpha_3 \varepsilon_{11}^0 + \alpha_4 \varepsilon_{22}^0, \quad a_3^{(3)} = \alpha_8 \varepsilon_{11}^0, \quad a_4^{(3)} = \alpha_6 \varepsilon_{11}^0,$$

$$\begin{aligned}
a_5^{(3)} &= \alpha_{11}\varepsilon_{11}^0 + \alpha_{12}\varepsilon_{22}^0, & a_6^{(3)} &= \alpha_{16}\varepsilon_{22}^0, & a_7^{(3)} &= \alpha_{15}\varepsilon_{22}^0, \\
a_1^{(4)} &= \alpha_{10}\varepsilon_{11}^0, & a_2^{(4)} &= \alpha_9\varepsilon_{11}^0, & a_3^{(4)} &= \alpha_{13}\varepsilon_{11}^0, \\
a_1^{(5)} &= \alpha_7\varepsilon_{11}^0, & a_2^{(5)} &= \alpha_2\varepsilon_{11}^0 + \alpha_1\varepsilon_{22}^0, & a_3^{(5)} &= \alpha_4\varepsilon_{11}^0 + \alpha_3\varepsilon_{22}^0, \\
a_4^{(5)} &= \alpha_9\varepsilon_{11}^0, & a_5^{(5)} &= \alpha_{12}\varepsilon_{11}^0 + \alpha_{11}\varepsilon_{22}^0, \\
a_1^{(6)} &= \alpha_{10}\varepsilon_{22}^0, & a_2^{(6)} &= \alpha_8\varepsilon_{11}^0, & a_3^{(6)} &= \alpha_{13}\varepsilon_{22}^0, \\
a_1^{(7)} &= \alpha_7\varepsilon_{11}^0, & a_2^{(7)} &= \alpha_{14}\varepsilon_{22}^0, & a_3^{(7)} &= \alpha_5\varepsilon_{22}^0, & a_4^{(7)} &= \alpha_6\varepsilon_{11}^0, \\
a_5^{(7)} &= \alpha_5\varepsilon_{11}^0, & a_6^{(7)} &= \alpha_{14}\varepsilon_{11}^0, \\
a_1^{(8)} &= \alpha_8\varepsilon_{11}^0, & a_2^{(8)} &= \alpha_5\varepsilon_{22}^0, & a_3^{(8)} &= \alpha_{13}\varepsilon_{22}^0, & a_4^{(8)} &= \alpha_6\varepsilon_{11}^0, \\
a_5^{(8)} &= \alpha_{11}\varepsilon_{11}^0 + \alpha_{12}\varepsilon_{22}^0, \\
a_1^{(9)} &= \alpha_7\varepsilon_{11}^0, & a_2^{(9)} &= \alpha_9\varepsilon_{11}^0, & a_3^{(9)} &= \alpha_{12}\varepsilon_{11}^0 + \alpha_{11}\varepsilon_{22}^0, \\
a_4^{(9)} &= \alpha_5\varepsilon_{11}^0, & a_5^{(9)} &= \alpha_{13}\varepsilon_{11}^0, \\
a_1^{(10)} &= \alpha_1\varepsilon_{11}^0 + \alpha_2\varepsilon_{22}^0, & a_2^{(10)} &= \alpha_9\varepsilon_{11}^0, & a_3^{(10)} &= \alpha_2\varepsilon_{11}^0 + \alpha_1\varepsilon_{22}^0, \\
a_4^{(10)} &= \alpha_8\varepsilon_{11}^0, & \text{and } a_5^{(10)} &= \alpha_{16}\varepsilon_{22}^0;
\end{aligned}$$

$$\begin{aligned}
\alpha_1 &= \frac{43389}{202376}, & \alpha_2 &= \frac{250084}{202376}, & \alpha_3 &= \frac{13241}{250084}, & \alpha_4 &= \frac{195816}{250084}, \\
\alpha_5 &= \frac{281752}{364649}, & \alpha_6 &= -\frac{364649}{71176}, & \alpha_7 &= -\frac{71176}{364649}, & \alpha_8 &= -\frac{64252}{22913}, \\
\alpha_9 &= -\frac{22913}{64252}, & \alpha_{10} &= -\frac{14539}{64252}, & \alpha_{11} &= -\frac{34085807}{14231592}, \\
\alpha_{12} &= \frac{4343048}{14231592}, & \alpha_{13} &= \frac{24431483}{21074656}, & \alpha_{14} &= -\frac{859}{217}, & \alpha_{15} &= \frac{48954}{62521}, \\
\alpha_{16} &= \frac{62521}{50594}, & \alpha_{17} &= \frac{209057}{250084}, & \text{and } \alpha_{18} &= \frac{293473}{202376};
\end{aligned}$$

$$\begin{aligned}
A_1^{(3)} &= 7537\varepsilon_{11}^0 + 13567\varepsilon_{22}^0 + 11927\varepsilon_{33}^0, \\
A_2^{(3)} &= 43389\varepsilon_{11}^0 + 250084\varepsilon_{22}^0 - 202376\varepsilon_{33}^0, \\
A_3^{(3)} &= -13241\varepsilon_{11}^0 - 195816\varepsilon_{22}^0 + 250084\varepsilon_{33}^0, \\
A_1^{(4)} &= 4187\varepsilon_{11}^0 + 32126(\varepsilon_{22}^0 - \varepsilon_{33}^0), \\
A_2^{(4)} &= 22913\varepsilon_{11}^0 + 64252\varepsilon_{22}^0, \\
A_3^{(4)} &= -14539\varepsilon_{11}^0 - 64252\varepsilon_{33}^0,
\end{aligned}$$

$$\begin{aligned}
A_1^{(5)} &= 13567\varepsilon_{11}^0 + 7537\varepsilon_{22}^0 + 11927\varepsilon_{33}^0, \\
A_2^{(5)} &= 250084\varepsilon_{11}^0 + 43389\varepsilon_{22}^0 - 202376\varepsilon_{33}^0, \\
A_3^{(5)} &= -195816\varepsilon_{11}^0 - 13241\varepsilon_{22}^0 + 250084\varepsilon_{33}^0, \\
A_1^{(6)} &= 4187\varepsilon_{22}^0 + 32126(\varepsilon_{11}^0 - \varepsilon_{33}^0), \\
A_2^{(6)} &= 64252\varepsilon_{11}^0 + 22913\varepsilon_{22}^0, \\
A_3^{(6)} &= -14539\varepsilon_{22}^0 - 64252\varepsilon_{33}^0, \\
A_1^{(7)} &= 859(\varepsilon_{11}^0 - \varepsilon_{22}^0), \\
A_2^{(7)} &= 859\varepsilon_{11}^0 + 217\varepsilon_{33}^0, \\
A_3^{(7)} &= -859\varepsilon_{22}^0 - 217\varepsilon_{33}^0, \\
A_1^{(8)} &= 4869401\varepsilon_{11}^0 - 4587649\varepsilon_{22}^0 - 364649\varepsilon_{33}^0, \\
A_2^{(8)} &= 34085807\varepsilon_{11}^0 - 126500463\varepsilon_{22}^0 + 119604872\varepsilon_{33}^0, \\
A_3^{(8)} &= 4869401(\varepsilon_{11}^0 - \varepsilon_{22}^0), \\
A_4^{(8)} &= 34085807\varepsilon_{11}^0 - 4343048\varepsilon_{22}^0 + 14231592\varepsilon_{33}^0, \\
A_5^{(8)} &= -24431483\varepsilon_{22}^0 + 21074656\varepsilon_{33}^0, \\
A_1^{(9)} &= 4587649\varepsilon_{11}^0 - 4869401\varepsilon_{22}^0 + 364649\varepsilon_{33}^0, \\
A_2^{(9)} &= 126500463\varepsilon_{11}^0 - 34085807\varepsilon_{22}^0 - 119604872\varepsilon_{33}^0, \\
A_3^{(9)} &= 4869401(\varepsilon_{11}^0 - \varepsilon_{22}^0), \\
A_4^{(9)} &= 24431483\varepsilon_{11}^0 - 21074656\varepsilon_{33}^0,
\end{aligned}$$

and

$$A_5^{(9)} = 4343048\varepsilon_{11}^0 - 34085807\varepsilon_{22}^0 - 14231592\varepsilon_{33}^0.$$

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Figure captions:

Fig. 1 Schematic of the correspondence between the Cartesian coordinate axes (x , y , and z) and crystallographic directions of the α -Mg matrix ($[2\bar{1}\bar{1}0]_\alpha$, $[01\bar{1}0]_\alpha$, and $[0001]_\alpha$), where θ is the angle between the vector $\mathbf{n}$ and z -axis, and ϕ is the angle between the projection of the vector $\mathbf{n}$ on the x - y plane and x -axis.

Fig. 2 Stress-free transformation strain conditions (ε_{11}^0 , ε_{22}^0 , and ε_{33}^0) for the formation of $(01\bar{1}0)_\alpha$ plate-shaped precipitates in the α -Mg matrix.

Fig. 3 Stress-free transformation strain conditions (ε_{11}^0 , ε_{22}^0 , and ε_{33}^0) for the formation of $(2\bar{1}\bar{1}0)_\alpha$ plate-shaped precipitates in the α -Mg matrix.

Fig. 4 (a) Orientation dependence of $B(\mathbf{n})$ when the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.014$, $\varepsilon_{22}^0 = 0.013$, and $\varepsilon_{33}^0 = 0.011$. The straight-line distance from the origin to the curvilinear surface of the white region corresponds to the magnitude of $B(\mathbf{n})$ normalized by $\bar{B}$. (b) and (c) are the x - z and x - y cross sections of (a), respectively.

Fig. 5 Schematic of the habit planes of a plate-shaped precipitate when the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.01$, $\varepsilon_{22}^0 = 0.01$, and $\varepsilon_{33}^0 = 0.002$. Arbitrary plate-shaped inclusions whose habit planes are perpendicular to the $(0001)_\alpha$ plane have a strain energy of the same magnitude. The zone axis of these habit planes is along the $[0001]_\alpha$ direction.

Fig. 6 Total energy E_{total} (i.e., the sum of the strain and interface energies) of a spheroidal inclusion as a function of the aspect ratio of the spheroid p . The inclusion volume is set as $V_0 = 4\pi r_0^3/3$, and the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.01$, $\varepsilon_{22}^0 = 0.01$, and $\varepsilon_{33}^0 = 0.002$. The total energy of the spheroidal inclusion is normalized by the total energy of a spherical inclusion with the same volume. Three different cases are shown in which the rotation axis of the spheroid is parallel to the $[2\bar{1}\bar{1}0]_\alpha$, $[01\bar{1}0]_\alpha$, or $[0001]_\alpha$ direction.

Fig. 7 Total energy E_{total} (i.e., the sum of the strain and interface energies) of a spheroidal inclusion as a function of the aspect ratio of the spheroid p . The inclusion volume is set as $V_0 = 4\pi r_0^3/3$, and the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.0007$, $\varepsilon_{22}^0 = 0.0007$, and $\varepsilon_{33}^0 = 0.002$. The total energy of the spheroidal inclusion is normalized by the total energy of a spherical inclusion with the same volume. Three different cases are shown in which the rotation axis of the spheroid is parallel to the $[2\bar{1}\bar{1}0]_\alpha$, $[01\bar{1}0]_\alpha$, or $[0001]_\alpha$ direction.

Fig. 8 Schematic of the habit planes of a plate-shaped precipitate when the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.01$, $\varepsilon_{22}^0 = 0.005$, and $\varepsilon_{33}^0 = 0.009$. Two habit planes are perpendicular to the $(01\bar{1}0)_\alpha$ plane, and the zone axis of the two habit planes (dashed line) is along the $[01\bar{1}0]_\alpha$ direction.

Fig. 9 Total energy E_{total} (i.e., the sum of the strain and interface energies) of a spheroidal inclusion as a function of the aspect ratio of the spheroid p . The inclusion volume is set as $V_0 = 4\pi r_0^3/3$ ((a) $r_0 = 50$ nm and (b) $r_0 = 500$ nm), and the stress-free transformation strain is assumed to be $\varepsilon_{11}^0 = 0.004$, $\varepsilon_{22}^0 = 0.008$, and $\varepsilon_{33}^0 = 0.003$. The total energy of the spheroidal inclusion is normalized by the total energy of a spherical inclusion with the same

volume. Three different cases are shown in which the rotation axis of the spheroid is parallel to the $[2\bar{1}\bar{1}0]_a$, $[01\bar{1}0]_a$, or $[0001]_a$ direction.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9 (a)

Figure 9 (b)