

Three-Dimensional Dynamic Calculation of the Equilibrium Shape of a Coherent Tetragonal Precipitate in Mg-Partially Stabilized Cubic ZrO₂

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The equilibrium shape of a tetragonal precipitate coherently embedded in a cubic matrix is examined in three dimensions by a computer simulation. Independent experimental data of Mg-partially stabilized ZrO₂ are used as the input parameters. The equilibrium shape is obtained by diffusional relaxation of an initially nonequilibrium spherical shape. The relaxation is described through a generalized field kinetic model which takes into account the transformation-induced elastic strain arising from a cubic \rightarrow tetragonal crystal lattice rearrangement. Without any a priori constraint on the geometry of the particle, the equilibrium shape is shown to be a rotation disk formed by two cones with the common base. It is far from the ellipsoidal shape assumed in the conventional analytical calculations based on Eshelby's model.

I. Introduction

A QUANTITATIVE theoretical prediction of the optimal shape of a low-symmetry precipitate coherently embedded in a high-symmetry matrix is an interesting and important problem of materials science. It has many applications in material processing and in service performance analysis, since the majority of high-performance structural materials in modern technology are two-phase or multiphase coherent composites of metal and ceramic systems. The coexisting phases usually have not only different compositions and structures, but also different point group symmetries, for example, cubic and tetragonal. A typical example is transformation-toughened partially stabilized zirconia (PSZ). It is a cubic solid solution at high temperatures. Upon cooling or aging at temperatures within the two-phase field of the cubic (*c*-) and tetragonal (*t*-) phases in the equilibrium phase diagram, it decomposes into a coherent two-phase mixture with the low-symmetry *t*-precipitates dispersed in the high-symmetry parent phase matrix. Under service conditions, e.g., in the presence of stress fields of propagating cracks, the *t*-particles are unstable with respect to further martensitic transformation into monoclinic phase particles.¹⁻³ This stress-induced martensitic transformation has a volume dilatation which may produce a back stress on the crack tip and hence toughen the material. Since particles of different morphology may have different stress fields associated with them and hence behave differently in the stress-induced martensitic transformation, a correct characterization of their shape is essential in the micromechanical analysis and property prediction.

Most of the existing theoretical analyses based on Eshelby's theory find the optimal shape of a coherent *t*-particle by minimizing the sum of interfacial and strain energies under a constraint that all adjusting shape changes keep the particle shape within a class of ellipsoidal forms.⁴ Although such an ellipsoidal particle shape approximation allows an analytical treatment of the problem, it can be misleading in predicting the micro-mechanical properties.⁵ Recently, computer simulation technique based on a generalized field kinetic model has been utilized to characterize the dynamic shape evolution of the coherent tetragonal precipitates in Mg-PSZ in two dimensions (2-D) without any constraint on particle shapes.⁶ It has been shown that the equilibrium shape in 2-D differs quite significantly from an ellipsoid. It is a rhombus bounded by facets. Recent bifurcation analysis based on total energy (the sum of strain and interfacial energies) minimization using a sharp interface approach yields a similar result.⁷ However, these 2-D studies can describe only an infinitely long cylindrical shape and yield no information in the third dimension. In reality, the tetragonal precipitates in Mg-PSZ are never cylindrical. They usually have a disklike shape with the smallest dimension along their *c*-axis.

In this paper, we have extended the 2-D field kinetic model developed in Ref. 6 into 3-D and applied it to examine the equilibrium shape of a single tetragonal precipitate coherently embedded in a cubic matrix. In the next section, we briefly discuss how the generalized field kinetic model can be used, free from any a priori constraint, to determine the equilibrium shape of a coherent precipitate which has an arbitrarily different point group symmetry from the matrix. For the details of the model, the readers should refer to references.⁶ We then set up a model system using the experimental data of Mg-PSZ. The obtained 3-D optimal shape is compared with the experimental observations.

II. Field Kinetic Equations

The field theory of phase transformation kinetics is a major advance in materials science. It allows a theoretical characterization of the dynamic evolution of microstructures during processing or in-service performance of advanced multiphase materials without any a priori assumptions on the microstructure and its evolution path.⁸ In this approach, an arbitrary two-phase morphology evolving with time is described through continuous fields of concentration $\{c(\mathbf{r})\}$ (characterizing the compositional heterogeneity) and/or structure order (SO) parameters $\{\eta_\alpha(\mathbf{r})\}$ (characterizing the structural heterogeneity), where \mathbf{r} is the coordinate and $\alpha = 1, 2, \dots, v$ numerates a complete set of SO parameters needed to characterize the structural heterogeneity. For example, a cubic \rightarrow tetragonal transformation is characterized by three SO parameters $\eta_1(\mathbf{r})$, $\eta_2(\mathbf{r})$, and $\eta_3(\mathbf{r})$, each of them describing the corresponding orientation variant of the tetragonal phase. The temporal evolution of these fields can be described by the time-dependent Ginzburg-Landau (TDGL) equations

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$$\frac{dc(\mathbf{r},t)}{dt} = M\nabla^2 \frac{\delta F}{\delta c(\mathbf{r},t)} \quad (1a)$$

$$\frac{\partial \eta_\alpha(\mathbf{r},t)}{\partial t} = -L \frac{\delta F}{\delta \eta_\alpha(\mathbf{r},t)} \quad (1b)$$

where M and L are kinetic constants characterizing the diffusional and structural relaxations, respectively, ∇ is the differential operator, and F is the total nonequilibrium free energy. The solution of these nonlinear field kinetic equations will yield all the information about the microstructure development during a phase transformation, including all the metastable and transient structures.

Although the field method is able to deal with arbitrary morphological pattern dynamics, there is a major limitation in the current formalisms: the transformation-induced elastic strain effect is generally not taken into account in them. This limitation drastically reduces the predicting power and realism of the theory because, in most cases, it is the accommodation of the coherency strain that dominates the microstructural development, e.g., particle shapes and spatial collective patterns. There have been several attempts to include the misfit strain effect into the field equations (e.g., Cahn⁹ for linearized equations and Nishimori and Onuki¹⁰ for nonlinearized equations). However, they were made only for a particular case of isostructural spinodal decomposition in cubic systems characterized by a sole concentration field. Recently, this method has been advanced to a more general model by (i) introducing the multi-component SO parameter $\eta_\alpha(\mathbf{r})$ and (ii) incorporating the transformation strain generated by the crystal lattice misfit between the product and parent phases as well as between different orientation domains of the low symmetry product phase.⁶ These advances make the model applicable to more general cases where, besides composition, structural rearrangement producing a low-symmetry phase with several orientation variants is involved.

One of the simplest applications of the coherent field kinetic model is determining the equilibrium shape of an arbitrary coherent precipitate without any constraint on its optimal shape. It follows from Eqs. (1a) and (1b) that when $c(\mathbf{r},t)$ and $\eta_\alpha(\mathbf{r},t)$ do not correspond to an equilibrium state, the variational derivatives of the total free energy with respect to them, $\delta F/\delta c(\mathbf{r},t)$ and $\delta F/\delta \eta_\alpha(\mathbf{r},t)$, which are the thermodynamic driving forces for the microstructure evolution, will have finite values and therefore they will drive the system toward the equilibrium state where $\delta F/\delta c(\mathbf{r},t)$ and $\delta F/\delta \eta_\alpha(\mathbf{r},t)$ vanish. Therefore, we may start from any reasonable initial guess of the equilibrium shape, e.g., an isotropic sphere, characterized by $c(\mathbf{r},0)$ and $\eta_\alpha(\mathbf{r},0)$. Then their relaxation toward equilibrium will automatically yield the optimal shape. To avoid the system stacking into possible metastable states, Langevin noise terms^{8,11} can be introduced into the TDGL equations.

The closed forms of Eqs. (1a) and (1b) are obtained if the total nonequilibrium free energy including the strain energy is formulated as a functional of $c(\mathbf{r})$ and $\eta_\alpha(\mathbf{r})$. Below, we first construct the free-energy functional for a generic two-phase system and then fit those input parameters that determine an equilibrium shape to the Mg-PSZ.

III. Model System and Input Parameters

If there are no external fields, the independent thermodynamic parameters determining the equilibrium shape of a coherent precipitate include the interfacial energy and the misfit strain energy. They enter the total nonequilibrium free energy in (1a) and (1b). The interfacial energy which is a part of the "chemical" free energy originates from a short-range atomic interaction. The "coarse-grained" representation of the chemical free energy for the cubic \rightarrow tetragonal transformation can be formulated as

$$F_0 = \int_V \left[\frac{1}{2} a_{ij} \nabla_i c \nabla_j c + \frac{1}{2} \sum_{\alpha=1}^3 b_{ij}(\alpha) \nabla_i \eta_\alpha \nabla_j \eta_\alpha + f(c, \eta_1, \eta_2, \eta_3) \right] d^3r \quad (2)$$

where a_{ij} and $b_{ij}(\alpha)$ are coefficients of the gradient terms which are responsible for the field continuity (nonlocal contribution to the free energy), i, j are indexes of Cartesian coordinates, and $f(c, \eta_1, \eta_2, \eta_3)$ is the local specific free energy. The integration in (2) is carried out over the entire system volume V .

Since we consider here a single particle problem, i.e., a situation where $\eta_1(\mathbf{r}) = \eta(\mathbf{r})$, $\eta_2(\mathbf{r}) = \eta_3(\mathbf{r}) = 0$, Eq. (2) can be simplified as

$$F_0 = \int_V \left[\frac{1}{2} a |\nabla c|^2 + \frac{1}{2} b |\nabla \eta|^2 + f(c, \eta) \right] d^3r \quad (3)$$

where the gradient energy coefficient matrices have been assumed to be isotropic:

$$\begin{cases} a_{ij} = a\delta_{ij} \\ b_{ij}(\alpha) = b\delta_{ij} \end{cases} \quad (4)$$

which provide an isotropic interfacial energy. The specific free energy at a given temperature can be approximated by the Landau free-energy expansion polynomial. A simple form for a first-order transition is

$$f(c, \eta) = \frac{1}{2} A(c - c')^2 + \frac{1}{2} B(c - c'')\eta^2 - \frac{1}{4} D\eta^4 + \frac{1}{6} G\eta^6 \quad (5)$$

where A, B, D , and G are positive constants with a dimension of energy, and c' and c'' are close to the equilibrium compositions of the c - and t -phases, respectively. These phenomenological constants should be chosen in such a way that the free energy (5) has a correct hypersurface in the c - η space. For example, it should yield an equilibrium two-phase mixture of c - and t -phases and the dependence of f on η should have a local minimum at $\eta = 0$ and two global minima at $\eta = \pm\eta_0$, where η_0 is the equilibrium SO parameter. These features are illustrated in Figs. 1(a) and (b). The invariance of f with respect to $\eta \rightarrow -\eta$ characterizes degeneracy of the free energy with respect to two antiphase domains of an orientation variant of the t -phase, which correctly represents the case of PSZ. A particular set of the constants $A = 80$, $B = 5.0$, $D = 0.5$, $G = 0.14$ (in the unit $k_B T$, where $T = 1420^\circ\text{C}$), $c' = 0.16$ and $c'' = 0.04$ has been chosen to meet the above geometrical requirement of the free-energy hypersurface and to fit the observed equilibrium compositions of Mg-PSZ. It provides equilibrium compositions $c_{\text{tet}} = 0.045$ for the t -phase and $c_{\text{cub}} = 0.155$ for the c -phase, which are close to the equilibrium compositions of Mg-PSZ at 1420°C .¹²

When the phenomenological constants in Eq. (5) are chosen, the parameter a in the gradient coefficient matrices (4) will dictate the value of interfacial energy caused by the concentration change at the interface between different phases and b will determine the value of interfacial energy caused by SO parameter change at the same interface. The latter also determines the interfacial energy between two orientation variants and between two antiphase domains of the tetragonal phase. Since we have considered a single-domain particle, there are no different orientation variants and antiphase domains in the system. Therefore, the parameter b contributes to the interfacial energy only. In this case, any choice of the coefficients a and b is good as long as they provide the required interfacial energy. For the sake of simplicity, we have chosen $a = b = 0.2$ in the unit $a_0^2 k_B T$, where a_0 is the length unit of the cubic computational unit cells (one grid length of the cubic mesh). The dimensional value of a_0 can be characterized by fitting the interfacial

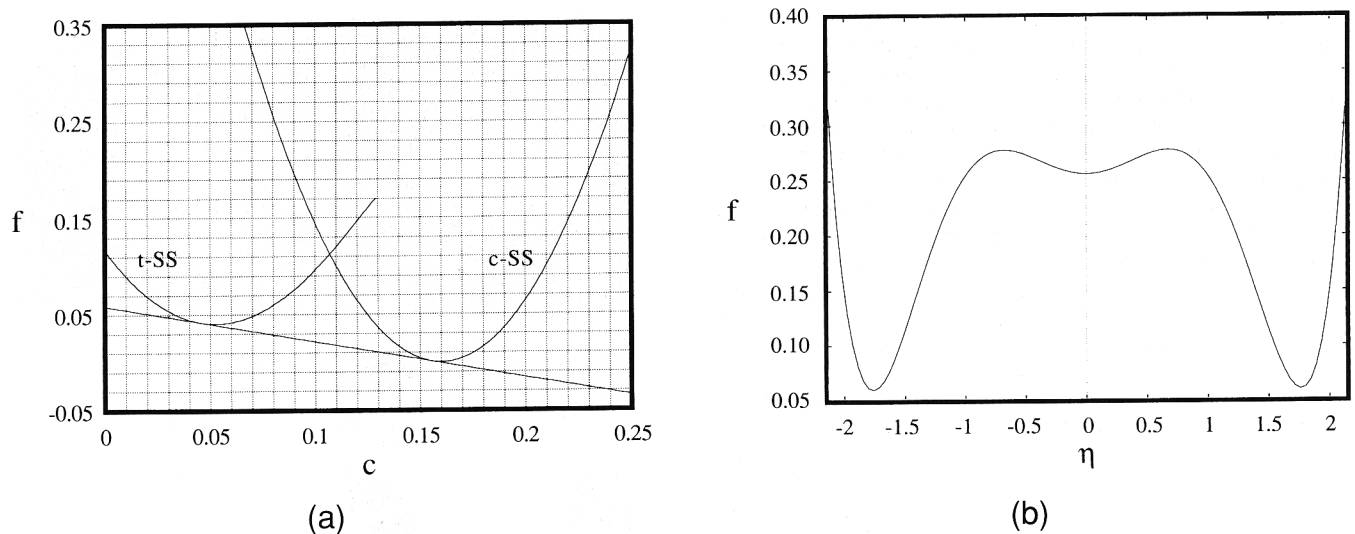


Fig. 1. (a) Specific free energy vs composition curves (on f - c plane) for both the tetragonal and cubic solid solutions calculated according to Eq. (1) with $\eta = \eta_0(c)$ (where η_0 is the equilibrium SO parameter at given c) and $A = 80.0$, $B = 0.8$, $C = 0.5$, $D = 0.14$, $G = 5.0$. (b) Specific free energy vs SO parameter curve (on f - η plane) at given composition.

energy obtained in the simulation into the experimental data. For example, with $\gamma_s = 150$ ergs/cm²,¹³ a_0 comes up to ~ 40 Å.

In the general strain energy analysis for inhomogeneous coherent solids proposed by Khachaturyan and Shatalov,¹⁴ the strain energy of an arbitrary coherent multiphase system for the homogeneous modulus case is expressed as a functional of the transformation-induced stress free strain $\epsilon_{ij}^0(\mathbf{r})$ which is presented through an arbitrary shape function $\theta_p(\mathbf{r})$, e.g.,

$$\epsilon_{ij}^0(\mathbf{r}) = \sum_{p=1}^v \theta_p(\mathbf{r}) \epsilon_{ij}^{00}(p) \quad (6)$$

where $\theta_p(\mathbf{r})$ equals unity if a point, \mathbf{r} , is within a new phase particle of type p and zero outside it, the tensor $\epsilon_{ij}^{00}(p)$ describes the stress-free transformation strain transforming the parent phase into the p th orientation variant of the low-symmetry product phase.

In fact, the stress-free strain Eq. (6) is formulated for the conventional description of a multiphase system, e.g., a coherent aggregate of internally homogeneous particles of constituent phases and their orientation variants with sharp interfacial boundaries between them. In the field approach, however, the multiphase mixture is described by continuous fields of concentration and SO parameters. To incorporate the strain energy into the field kinetic equations, we have to modify the theory¹⁴ by expressing the stress-free strain through the continuum fields of $c(\mathbf{r})$ and/or $\eta(\mathbf{r})$. Since the strain in ZrO₂ is predominantly caused by the SO parameter heterogeneity, e.g., the lattice misfit is caused by the symmetry breaking "soft" displacive modes, we may express the stress-free strain through $\eta(\mathbf{r})$, i.e.,

$$\epsilon_{ij}^0(\mathbf{r}) = \sum_{p=1}^v \eta_p^2(\mathbf{r}) \epsilon_{ij}^{00}(p) \quad (7)$$

where the fact that the $\eta \rightarrow -\eta$ transition (e.g., an antiphase domain shift) does not affect the transformation strain in PSZ has been taken into account.

Keeping in mind the correspondence between $\eta_p^2(\mathbf{r})$ and $\theta_p(\mathbf{r})$ in Eqs. (6) and (7) and following the same line of reasoning as in Ref. 14, we can express the strain energy as a functional of the SO parameter fields

$$E_{el} = \frac{1}{2} \sum_{pq} \int \frac{d^3k}{(2\pi)^3} B_{pq} \left(\frac{\mathbf{k}}{k} \right) \{ \eta_p^2(\mathbf{r}) \}_k \{ \eta_q^2(\mathbf{r}) \}_k^* \quad (8)$$

where $\{ \eta_p^2(\mathbf{r}) \}_k$ is the Fourier transform of $\eta_p^2(\mathbf{r})$, $\{ \eta_q^2(\mathbf{r}) \}_k^*$ is the complex conjugate of $\{ \eta_q^2(\mathbf{r}) \}_k$ and

$$B_{pq}(\mathbf{e}) = c_{ijkl} \epsilon_{ij}^{00}(p) \epsilon_{kl}^{00}(q) - e_i \sigma_{ij}^0(p) \Omega_{jk}(\mathbf{e}) \sigma_{kl}^0(q) e_l \quad (9)$$

$\mathbf{e} = \mathbf{k}/k$ is a unit vector in the reciprocal space and e_i is its i th component, c_{ijkl} is the elastic moduli tensor, $\sigma_{ij}^0(p) = c_{ijkl} \epsilon_{kl}^{00}(p)$, and $\Omega_{ij}(\mathbf{e})$ is a Green function tensor which is inverse to the tensor $\Omega(\mathbf{e})_{ij}^{-1} = c_{ijkl} e_k e_l$. The sign f in Eq. (9) indicates that a volume of $(2\pi)^3/V$ about $k = 0$ is excluded from the integration. When V is large, this exclusion defines the "principle value" of the integral.

It can be seen from Eqs. (8) and (9) that the function $B_{pq}(\mathbf{e})$ carries all the information on the elastic properties of a system and the crystallography of the phase transformation taking place. It is actually the Fourier transform of the strain-induced interaction potential, $W_{el}^{pq}(\mathbf{r} - \mathbf{r}')$, between finite elements of particles of type p and q at points \mathbf{r} and \mathbf{r}' . It should be mentioned that $B_{pq}(\mathbf{k}/k)$ has a singularity at $\mathbf{k} = 0$, since its limit at $\mathbf{k} \rightarrow 0$ depends on the direction of \mathbf{k} . This singularity yields a $1/r^3$ dependence of its back Fourier transform and hence is responsible for the dipole-dipole-like infinitely long-ranged asymptotic behavior of the strain-induced interaction $W_{el}^{pq}(\mathbf{r})$. Such an interaction, in principle, cannot be reduced to the gradient terms in the continuum limit. Therefore, the strain energy is very different from the interfacial energy. It is a bulk free energy which is proportional to the particle volume while the interfacial energy is proportional only to the total interfacial area. The strain energy is also different from the bulk chemical free energy because it is morphology-dependent. Owing to these particular features, the shape of a coherent particle is volume-dependent, and the equilibrium shape in a coherent system is actually an equilibrium shape at fixed volume.

The elastic constants and lattice parameters of Mg-PSZ at 1420°C:¹² $c_{11} = 3.08$, $c_{12} = 0.69$, $c_{44} = 0.36$ (10^{12} erg/cm²) and $a_c = 5.094$, $a_t = 5.091$, and $c_t = 5.204$ (Å) are employed. The kinetic constants M and L are not important in determining an equilibrium shape, since they only affect the time to reach the equilibrium shape, but not the equilibrium shape itself. We have defined a reduced time $\tau = t(Lk_B T)$ in the simulation and the ratio $M/(La_0^2)$ is fixed to 0.4. With those chosen parameters, the kinetic equations (1a) and (1b) are solved numerically using their Fourier space (reciprocal space) representation for a 3-D model system consisting of $64 \times 64 \times 64$ mesh points of a cubic grid. The system size is $64 \times a_0 \sim 0.25$ μm . Periodic boundary conditions are applied along all three dimensions in the simulation.

IV. Results and Discussion

We start with a t -particle of equilibrium composition and SO parameter coherently embedded in an equilibrium c -matrix. It

has initially a spherical shape. Its size is $30a_0$ in diameter. The c -axis of the particle is directed along the [001] vertical direction. The spherical shape is the equilibrium shape for a stress-free particle in the system since, as has been mentioned before, the form of the gradient terms and the choice of the gradient energy coefficient provide an isotropic interfacial energy. It is also a good approximation of particle shapes at initial stages of precipitation when particles are small and the interfacial energy plays a more important role in the energy balance. However, the spherical shape is certainly a non-equilibrium shape for the misfitting particle at the given size considered here. According to Eqs. (1a) and (1b), the initial nonequilibrium spherical shape characterized by $c(\mathbf{r},0)$ and $\eta(\mathbf{r},0)$ should gradually evolve into their equilibrium configurations determined by the interplay between the isotropic interfacial energy and the anisotropic strain energy. Since such a shape relaxation is a spontaneous process, the total free energy of the system continuously decreases in our simulation. When the total free energy change with time reaches a plateau, we assume that the particle shape has reached the equilibrium shape.

The equilibrium shape obtained in this way for the given particle size and given set of material parameters is shown in Fig. 2. It is visualized by an iso-SO parameter plot. The three cross sections of the particle by (100), (010), and (001) planes are given in Figs. 3(a–c). They are visualized through the shades of gray in accordance with the SO parameter field $\eta(\mathbf{r})$; i.e., the completely dark regions represent $\eta(\mathbf{r}) = 0$, which denotes the equilibrium c -matrix while completely white ones represent $\eta(\mathbf{r}) = \eta_0$, which denotes the equilibrium t -particle. The steps shown on the particle are due to the fact that the scale of the mesh used in the simulation is commensurable with the particle size. It can be readily seen from these figures that the predicted optimal shape is far from an ellipsoid as assumed in the conventional analytical treatments. In fact, it is a rotation disk formed by two cones with the common base (see also the schematic drawing in Fig. 3(d)). The rotation axis coincides with the c -axis direction of the t -particle and is parallel to the [001] direction of the cubic phase matrix. Along this direction, the lattice misfit between the t -precipitate and the c -matrix is maximum, and the t -particle has its minimum dimension.

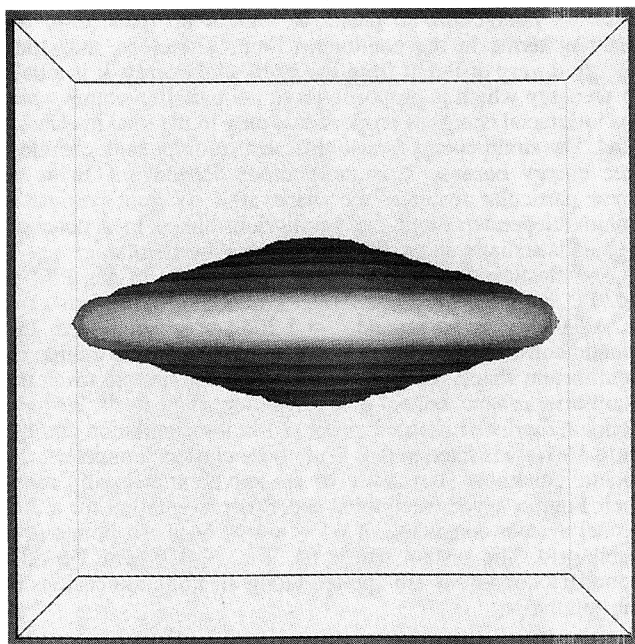


Fig. 2. Equilibrium shape of a tetragonal particle coherently embedded in a cubic matrix of Mg-PSZ at fixed size characterized by an interfacial-to-strain energy ratio 1.1.

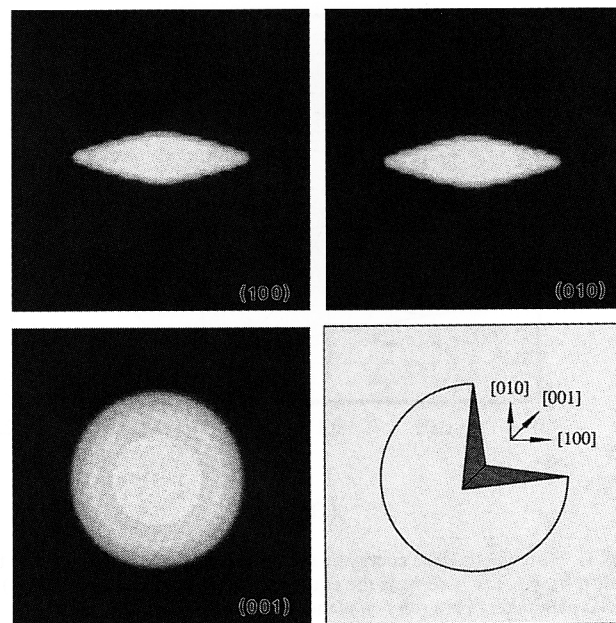


Fig. 3. (a–c) Cross sections of the tetragonal particle shown in Fig. 2 by (100), (010), and (001) planes. (d) Schematic drawing of the rotation disklike particle shape.

This simulation prediction is in agreement with electron microscope observations^{12,13,15,16} which have shown that the precipitates in Mg-PSZ have a faceted lenslike shape rather than ellipsoidal shape. The (100) and (010) cross sections of the particle shown in Figs. 3(a) and (b) practically coincide with the one reviewed by TEM using a (001) foil containing t -particles of similar sizes.¹⁶ They also agree well with our 2-D simulation predictions.⁶

It should be mentioned that if the initial configuration is far from equilibrium, the particle may reach its equilibrium shape through a different dynamic evolution path. For example, a transient concave shape and “splitting” pattern have been observed in the simulation when we start from a highly non-equilibrium shape, a cylinder of $r/h = 1$, where r is the radius and h is the height of the cylinder. Instead of gradual evolving, the cylinder initially splits into two particles whose shapes are much closer to the equilibrium one. This configuration is, however, not the equilibrium one, since it has higher energy than the equilibrium single particle obtained in Fig. 2. If we wait long enough, the two transient particles should coalesce into a single particle of the equilibrium shape. The transient concave particle shape and splitting phenomena have also been obtained in our simulation studies of particle shape evolution in superalloys.^{6,17} They are also observed experimentally.^{18,19}

It should also be emphasized that the result obtained above is confined to the given particle size, since the equilibrium shape of a coherent particle is size-dependent. Our previous 2-D simulation study has shown that, when the particle is relatively small, the equilibrium shape in 2-D is a rhombus with smoothly curved interfaces and corners. As the particle size increases, the aspect ratio of the particle increases and its interfaces become straight and corners become sharp. According to the 2-D energetic analysis,⁷ a shape bifurcation where the rhombus spontaneously transforms into a lower symmetry elongated shape should be expected when the size of the t -particle exceeds a certain critical value.

The strain-induced and diffusional multiparticle interactions are not considered in this study. As has been shown by both the TEM micrographs^{2,12,13} and our 2-D simulations,⁶ the shape of the t -particle in Mg-PSZ can be strongly influenced by the interactions between particles. It should be interesting to investigate how the strain accommodation among the three orientation variants of the t -precipitates affect the particle shape and their spatial distribution. Corresponding work is under way.

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References

- ¹R. C. Garvie, R. H. Hannink, and R. T. Pascoe, "Ceramic Steel?," *Nature (London)*, **258** [5537] 703–704 (1975).
- ²D. L. Porter and A. H. Heuer, "Mechanisms of Toughening Partially Stabilized Zirconia (PSZ)," *J. Am. Ceram. Soc.*, **60**, 183 (1977).
- ³For a review see A. H. Heuer, "Transformation Toughening in ZrO₂-Containing Ceramics," *J. Am. Ceram. Soc.*, **70**, 689 (1987).
- ⁴W. C. Johnson and J. W. Cahn, "Elastically Induced Shape Bifurcations of Inclusions," *Acta Metall.*, **32**, 1925 (1984).
- ⁵S. S. Rao, T. Tsakalakos, and W. R. Cannon, "Stress Distributions in Ceramic Composites Containing Faceted Inclusions," *J. Am. Ceram. Soc.*, **75**, 1807 (1992).
- ⁶(a) Y. Wang, "Theoretical Characterization and Modeling of Microstructure Development during Coherent Phase Transformations in Metals and Ceramics"; Ph.D. Dissertation. Rutgers, the State University of New Jersey, New Brunswick, New Jersey, May 1995; (b) Y. Wang, H. Y. Wang, L. Q. Chen, and A. G. Khachaturyan, "Shape Evolution of a Coherent Tetragonal Precipitate in Partially Stabilized Cubic ZrO₂: A Computer Simulation," *J. Am. Ceram. Soc.*, **76**, 3029 (1993); (c) "Microstructural Development of Coherent Tetragonal Precipitates in Mg-PSZ, A Computer Simulation," *ibid.*, **78**, 657 (1995).
- ⁷M. E. Thompson, C. S. Su, and P. W. Voorhees, "The Equilibrium Shape of a Misfitting Precipitate," *Acta Metall. Mater.*, **42**, 2107 (1994).
- ⁸For a general review see J. D. Gunton, M. S. Miguel, and P. S. Sahni, "The Dynamics of First-order Phase Transitions"; pp. 267–466 in *Phase Transitions and Critical Phenomena*. Edited by C. Domb and J. L. Lebowitz, Vol. 8. Academic Press, New York, 1983.
- ⁹J. W. Cahn, "On Spinodal Decomposition in Cubic Crystals," *Acta Metall.*, **10**, 179 (1962).
- ¹⁰H. Nishimori and A. Onuki, "Pattern Formation in Phase-Separating Alloys with Cubic Symmetry," *Phys. Rev. B*, **42**, 980 (1990).
- ¹¹L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Vol. 5 of Course of Theoretical Physics, 3rd ed., revised and enlarged by E. M. Lifshitz and L. P. Pitaevskii, translated from Russian by J. B. Sykes and M. J. Kearsley. Pergamon Press, New York, 1980.
- ¹²C. A. Bateman and M. R. Notis, "Coherency Effects during Precipitate Coarsening in Partially Stabilized Zirconias," *Acta Metall. Mater.*, **40**, 2413 (1992).
- ¹³V. Lanteri, T. E. Mitchell, and A. H. Heuer, "Morphology of Tetragonal Precipitates in Partially Stabilized ZrO₂," *J. Am. Ceram. Soc.*, **69**, 564 (1986).
- ¹⁴A. G. Khachaturyan and G. A. Shatalov, "Elastic-Interaction Potential of Defects in a Crystal," *Sov. Phys. Solid State*, **11**, 118 (1969); see also the monograph *Theory of Structural Transformations in Solids*, Wiley, New York, 1983.
- ¹⁵L. H. Schonlein, "Microstructural Studies of an Mg-PSZ"; Ph.D. Thesis. Case Western Reserve University, Cleveland, OH, 1982.
- ¹⁶M. Ruhle and W. M. Kriven, "Analysis of Strain around Tetragonal and Monoclinic Zirconia Inclusions"; pp. 1579–73 in Proceedings of International Conference on Solid → Solid Phase Transformations. Edited by H. I. Aaronson, D. E. Laughlin, R. F. Sekerka, and C. M. Wayman. The Metallurgical Society of AIME, Warrendale, PA, 1982.
- ¹⁷(a) Y. Wang, L. Q. Chen, and A. G. Khachaturyan, "Shape Evolution of a Precipitate during Strain-Induced Coarsening: a Computer Simulation," *Scr. Metall. Mater.*, **25**, 1387 (1991); (b) "Kinetics of Strain-Induced Morphological Transformation in Cubic Alloys with a Miscibility Gap," *Acta Metall. Mater.*, **41**, 279 (1993); (c) Y. Wang and A. G. Khachaturyan, "Shape Instability during Precipitate Growth in Coherent Solids," *ibid.*, **43**, 1837 (1995); (d) "Microstructural Evolution during the Precipitation of Ordered Intermetallics in Multi-particle Coherent System," *Philos. Mag. A*, 1995 (in press).
- ¹⁸(a) T. Miyazaki, H. Imamura, and T. Kozaki, "The Formation of γ' Precipitate Doublets in Ni–Al Alloys and their Energetic Stability," *Mater. Sci. Eng.*, **54**, 9 (1982); (b) M. Doi, T. Miyazaki, and T. Wakatsuki, "The Effect of Elastic Interaction Energy on the Morphology of γ' Precipitates in Ni-based Alloys," *ibid.*, **67**, 247 (1984).
- ¹⁹Y. S. Yoo, D. Y. Yoon, and M. F. Henry, "The Effect of Elastic Misfit Strain on the Morphological Evolution of γ' -Precipitates in a Model Ni-based Superalloy," *Met. Mater.*, **1**, 47 (1995). □