Phase-field modeling of $\gamma/\gamma''$ microstructure formation in Ni-based superalloys with high $\gamma''$ volume fraction

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The excellent mechanical properties of the Ni-based superalloy IN718 mainly result from coherent $\gamma''$ precipitates. Due to a strongly anisotropic lattice misfit between the matrix and the precipitate phase, the particles exhibit pronounced plate-shaped morphologies. Using a phase-field model, we investigate various influencing factors that determine the equilibrium shapes of $\gamma''$ precipitates, minimizing the sum of the total elastic and interfacial energy. Upon increasing precipitate phase fractions, the model predicts increasingly stronger particle-particle interactions, leading to shapes with significantly increased aspect ratios. Matching the a priori unknown interfacial energy density to fit experimental $\gamma''$ shapes is sensitive to the phase content imposed in the underlying model. Considering vanishing phase content leads to $30\%$ lower estimates of the interfacial energy density, as compared to estimates based on realistic phase fractions of $12\%$. We consider the periodic arrangement of precipitates in different hexagonal and rectangular superstructures, which result from distinct choices of point-symmetric and periodic boundary conditions. Further, non-volume conserving boundary conditions are implemented to compensate for strains due to an anisotropic lattice mismatch between the $\gamma$ matrix and the $\gamma''$ precipitate. As compared to conventional boundary conditions, this specifically tailored simulation configuration does not conflict with the systems periodicity and provides substantially more realistic total elastic energies at high precipitate volume fractions. The energetically most favorable superstructure is found to be a hexagonal precipitate arrangement.

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INTRODUCTION

Ni-based superalloys have various applications at elevated temperatures, especially in stationary gas turbines and airplane engines. The main strengthening mechanism, which makes these alloys applicable for high temperatures is particle strengthening by coherent precipitations [1]. Apart from the most prominent case, the $\gamma'$ strengthening of Ni-based superalloys for turbine blade materials, a series of alloys exist that are mainly strengthened by the tetragonal metastable $\gamma''$ phase. These Nb-containing alloys, such as the well-known IN718, can be cast, forged, machined and welded which renders them ideal candidates for industrial applications.

As IN718 contains up to $6\%$ of the cubic $L1_2$ phase $\gamma'$, several authors modified its composition in order to increase the volume fraction of $\gamma''$ phase and to get rid of $\gamma'$ precipitates while maintaining the composition of the matrix [2–5]. Table I shows the nominal composition of IN718 and a derivative IN718M without $\gamma'$ forming elements. Recent studies aim at deliberate co-precipitation of $\gamma'$ and $\gamma''$ to exploit ripening inhibiting effects [6, 7] and a dual lattice microstructure [8, 9]. IN718 powders also gain importance for additive manufacturing in the industrial environment [10–13]. It was recently found that alloys containing only one orientational variant of $\gamma''$, a so-called single-variant microstructure, can be used to tailor creep resistant materials [14].

Table I. Nominal composition in wt. % of IN718 and its derivative IN718M together with the measured composition in the Nb-rich region of IN718M as shown in Figure 1a).

| Composition in wt. % | Ni | Cr | Nb | Mo | Fe | Al | Ti |
|----------------------|----|----|----|----|----|----|----|
| IN718 nominal max.   | 55.0 | 21.0 | 5.5 | 3.3 | bal. | 0.8 | 1.2 |
| IN718 nominal min.   | 50.0 | 17.0 | 4.8 | 2.8 | bal. | 0.2 | 0.7 |
| IN718M nominal       | 58.0 | 18.0 | 5.0 | 3.0 | bal. | –   | –   |
| IN718M measured      | 56.8 | 17.6 | 6.6 | 3.2 | 15.8 | –   | –   |

The shapes and spatial arrangements of coherent misfitting precipitates have been modeled assuming a single precipitate embedded in infinite matrix [15–21]. The influence of elastic inhomogeneity [22] and periodic arrangements of precipitates with higher precipitate volume fractions [23] on precipitate shapes were studied using the boundary integral method. Comparison of simulated precipitate shapes to experimentally observed microstructures can be used to obtain realistic values of the interfacial energy density [24–26].

The phase-field method is widely considered to be a powerful tool for modeling solidification as well as solid-state phase transformations based on a diffuse descrip-

Figure 1a) shows a scanning electron microscope (SEM) image of a $\gamma/\gamma''$ microstructure in IN718M after homogenization at 1423 K for 2h. The precipitates are found in the Nb-rich interdendritic region. Table I also shows the local composition measured by energy-dispersive x-ray spectroscopy. The precipitates are arranged regularly in three spatial orientations perpendicular to one another and show a plate-shaped morphology. The volumetric $\gamma''$ phase fraction is $\geq 12\%$. Figure 1b) shows a dark-field transmission electron microscope (TEM) image of $\gamma''$ precipitates in IN718M.
now distinguish two lattice parameters $a_{\gamma''}$ and $c_{\gamma''}$, the latter being also referred to as the tetragonal axis. The plate normal of the precipitate is always parallel to the $c_{\gamma''}$ direction.

Coherent precipitation of $\gamma''$ in a $\gamma$ matrix is possible due to the relations

$$
\begin{align}
    a_{\gamma''} & \approx a_{\gamma} , \\
    c_{\gamma''} & \approx 2a_{\gamma} ,
\end{align}
$$

when

$$
\langle 100 \rangle \gamma \parallel \langle 100 \rangle \gamma''.
$$

This means that there are three possible orientational variants in which the tetragonal phase can coherently precipitate (see Figure 1) [47]. Note that Equation (1) states that there is a misfit of the lattice parameters that leads to strains when lattice coherency is kept. Two distinguishable misfit strains $\varepsilon_1$ and $\varepsilon_3$ in $a_{\gamma''}$ and $c_{\gamma''}$ direction, respectively, can be found.

Figure 2 shows a schematic drawing of a $\gamma''$ precipitate. The precipitate is depicted as an oblate spheroid with two major and a minor half axis $R$ and $r$, respectively. The orientational relations given in Equation (2) are depicted at the interface. To experimentally quantify the shape of $\gamma''$ precipitates one usually takes the aspect ratio that is defined as the ratio $R/r$ or, for non-elliptical precipitates the ratio of the plate diameter to its thickness. Usually, $\gamma''$ precipitates exhibit major radii of less than 130 nm and reportedly start to lose full coherency at major radii larger than 25 nm [25, 39, 48, 49].

**Elastic constants**

General elastic behavior is described by the tensor of elasticity $C_{ijkl}$. In this work, we use the tensor of elastic-

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**THE $\Gamma/\Gamma''$ MICROSTRUCTURE IN NI-BASED SUPERALLOYS**

The ordered D0$_{22}$ phase $\gamma''$ has a body-centered tetragonal (bct) crystallographic structure and is of the stoichiometric type Ni$_3$Nb. In an fcc matrix, it forms distinctive plate-shaped precipitates. The face-centered cubic (fcc) unit cell of the matrix phase $\gamma$ can be described by a single lattice parameter $a_{\gamma}$ that is the distance between two atom sites along a $\langle 100 \rangle$ direction. The bct unit cell of the $\gamma''$ phase can be made up by two fcc unit cells stacked on top of each other with the central atom site and the corner atom sites being Nb atoms. One can
ity in Voigt notation $C_{ij}$. This is a reduction to a $6 \times 6$ tensor that is not invariant under rotation. The cubic $\gamma$ and the tetragonal $\gamma''$ phase both exhibit anisotropic elastic properties due to their crystallographic symmetry. A set of three independent elastic constants is needed to describe cubic anisotropy ($C_{11}$, $C_{12}$, $C_{44}$) and six are needed for tetragonal anisotropy, respectively ($C_{11}$, $C_{33}$, $C_{12}$, $C_{13}$, $C_{44}$, $C_{66}$). Isotropic elasticity is described by a set of two independent constants with $C_{11} = 2C_{44} + C_{12}$.

In this work we use experimental data generated by resonance ultrasound spectroscopy (RUS) for polycrystalline (isotropic) and single crystal (anisotropic) samples of IN718. We assume that matrix and precipitates in IN718 and IN718M have comparable elastic properties. For the $\gamma''$ phase data from a first-principles study was used [50, 51]. This data is valid at 0 K, therefore, an estimate about temperature dependence has to be made. Due to the lack of experimental data, we propose to assume the same temperature dependence for all elastic constants considered, as it was already done by Moore et al. [52]. In this work, we assume a linear temperature dependence of the elastic constants

$$C_{ij}(T) = C_{ij}^{0K}(1 - \beta \Delta T),$$

where $T$ is the temperature, $C_{ij}^{0K}$ is an elastic constant at 0K and $\beta$ is the coefficient of temperature dependence. To determine $\beta$, experimental data for pure Nickel from 0 K to room temperature is used [53, 54]. For higher temperatures, we assume the same temperature dependence as it was determined for a $\gamma'$ single crystal (Ni-Al23-Ti1-Ta1) via RUS [55]. We find $\beta$ to be $2.3 \cdot 10^{-4}$ K$^{-1}$. Table II shows the extrapolated elastic constants of $\gamma''$ at 998 K. Elastic homogeneity is given when matrix and precipitate have the same tensor of elasticity ($C''_{ij} = C_{ij}^{\alpha}$).

The elastic constants of a single crystal alloy composed of $N$ coherent phases can be estimated by a simple rule of mixture

$$\bar{C}_{ij} = \sum_{\alpha} C_{ij}^{\alpha} V_{\alpha},$$

where $\bar{C}_{ij}$ is an elastic constant of the alloy, $C_{ij}^{\alpha}$ is the elastic constant of phase $\alpha$ and $V_{\alpha}$ is the volume fraction of $\alpha$. Knowing the elastic properties for all but one phase and for the alloy itself, it is possible to estimate the tensor of elasticity for the remaining phase. In the case of $\gamma''$ precipitates in a cubic matrix, the three orientational variants appear statistically. The tensor of elasticity of such an alloy maintains cubic symmetry. To find the tensor of elasticity, with cubic symmetry, for a mixture of all three orientation variants $\bar{C}_{ij}^{\gamma''}$ of the $\gamma''$ phase, we apply the modified mixture rule

$$\bar{C}_{ij}^{\gamma''} = \left(2C_{11}^{\gamma''} + C_{33}^{\gamma''}\right) / 3$$

and

$$\bar{C}_{ij}^{\gamma''} = \left(C_{12}^{\gamma''} + 2C_{13}^{\gamma''}\right) / 3$$

and

$$\bar{C}_{ij}^{\gamma''} = \left(2C_{44}^{\gamma''} + C_{66}^{\gamma''}\right) / 3.$$  

Having estimated the complete tensors of elasticity for the IN718M alloy and the $\gamma''$ phase, the anisotropic tensor of elasticity of the matrix can be calculated using Equation (4) and (7). In Table II also a stiffness contrast $C''_{ij} / C_{ij}^{\alpha}$ is given. In the case of anisotropic elasticity, we apply the mixture rule in Equation (7) to compare the respective tensors of elasticity. We report a mean value as the different elastic constants show different stiffness contrasts.

To evaluate the influence of inhomogeneous stiffness of the phases and of crystallographic anisotropy on the precipitate shapes, we use different sets of elastic constants. Phase-independent isotropic elastic properties leave only the anisotropic lattice misfit to determine the precipitate shape. Phase-wise isotropic data allows to observe the influence of elastic inhomogeneity. Individual cubic and tetragonally anisotropic phase data describes the elastic properties of the system in the most comprehensive way.

| elastic constants in GPa | contrast $C''_{ij} / C_{ij}^{\alpha}$ |
|--------------------------|--------------------------------------|
| $C_{11}$ | $C_{33}$ | $C_{12}$ | $C_{13}$ | $C_{44}$ | $C_{66}$ | $C''_{ij} / C_{ij}^{\alpha}$ |
| homogen.\(^1\) | 242 | 120 | 61 | $< 1.1$ |
| matrix\(^3\) | 240 | 120 | 60 |
| $\gamma''$ phase\(^4\) | 250 | 120 | 65 |
| homogen.\(^1\) | 205 | 145 | 90 | 1.0 |
| matrix\(^3\) | 200 | 150 | 90 |
| $\gamma''$ phase\(^2\) | 220 | 240 | 140 | 120 | 88 | 87 | $\approx 0.9$ |

Table II. Elastic constants at 998 K used in this work. Data for the individual phases and for an elastically homogeneous system ($C''_{ij} = C_{ij}^{\alpha}$) are provided as well as isotropic and anisotropic data sets to evaluate respective effects separately. Values of a mean stiffness contrast $C''_{ij} / C_{ij}^{\alpha}$ are provided. Data is generated via: \(^1\)resonance ultrasound spectroscopy, \(^2\)first-principles calculations [50, 51] and Equation (3) \(^3\)Equation (4) \(^4\)Equation (7).

All evaluations of the elastic moduli of the phases based Equation (4) are dependent on the volume fraction $V_{\alpha}$. In this work, we assume a $\gamma''$ volume fraction of 12% which is in accordance with previously reported values [56, 57] and higher than it was calculated using the Thermo-Calc software with the TCNi8 database.
Anisotropic lattice misfit

Due to the two distinguishable lattice parameters $a$ and $c$ in $\gamma''$ and the strict orientation relation of the coherent interface in a $\gamma/\gamma''$ microstructure the stress-free transformation strain $\varepsilon_0^{0}$ exhibits a tetragonal symmetry. In Voigt notation, this misfit strain tensor $\varepsilon_0$ of the $\gamma''$ phase is

$$\varepsilon_0 = (\varepsilon_1, \varepsilon_1, \varepsilon_3, 0, 0, 0)^T,$$  \hfill (8)

with the two distinguishable dilatational misfit strains $\varepsilon_1$ and $\varepsilon_3$. Those are calculated from the experimentally determined lattice parameters of the phases via

$$\varepsilon_1 = \frac{a_{\gamma''} - a_{\gamma}}{a_{\gamma}}, \quad \varepsilon_3 = \frac{c_{\gamma''} - 2a_{\gamma}}{2a_{\gamma}}.$$  \hfill (9)

Note that in the denominator we find only the lattice parameter of the matrix. This is because we define the eigenstrain of the matrix to be zero. The lattice parameters of an IN718 matrix and of the $\gamma''$ precipitates were measured by Slama et al. [47, 49] using X-ray diffractometry (XRD) for samples aged at 953K and 1023K after quenching. Lattice parameters were also measured using neutron diffraction [58]. Measured lattice parameters and corresponding misfit strains are given in Table III. Other measurements of the lattice parameters in IN718 show similar misfits [4, 48, 59–62]. Note that the absolute value of $\varepsilon_3$ is high compared to $\gamma'$ precipitates ($|\varepsilon_3| \approx -1 \ldots -3 \cdot 10^{-3}$ [63]) but similar for both XRD and neutron diffraction. On the other hand, the values of $\varepsilon_1$ differ strongly. The misfit ratio $\varepsilon_3/\varepsilon_1$ is one magnitude larger for neutron diffraction measurements than for the XRD measurements.

Both measurements, however, determined the in-situ constrained misfit that is the lattice misfit superimposed by elastic deformation of the material. A more suitable input parameter would be the unconstrained misfit that is the misfit calculated from lattice parameters of strain-free bulk samples of the phases. The unconstrained misfit can notably differ from the constrained misfit [64, 65].

| source | lattice param. in pm | misfit in $10^{-3}$ | $\varepsilon_1$ | $\varepsilon_3$ | $\varepsilon_3/\varepsilon_1$ |
|--------|----------------------|---------------------|----------------|----------------|------------------|
| [47, 49] | 359.5 | 361.4 | 742.1 | 5.29 | 32.1 | 6.1 |
| [58] | 359.8 | 360.0 | 743.8 | 0.56 | 33.6 | 60.0 |

Table III. Lattice parameters from literature for an IN718 matrix and $\gamma''$ precipitates. Misfit strains are given according to Equation (9) as well as the respective misfit ratio $\varepsilon_3/\varepsilon_1$. 

PHASE-FIELD MODELING OF EQUILIBRIUM PRECIPITATE SHAPES

The phase-field model for the simulation of solid-phase precipitation in multicomponent alloys is based on the following phenomenological potential functional [35, 66, 67].

$$\Omega = \int_V \omega (\varphi, \{\partial_i \varphi\}, \{\partial_k u_k\}) \, dV,$$  \hfill (10)

where $\partial_i$ denotes an abbreviation for the partial derivative with respect to the spacial directions $i = x, y, z$, e.g. $\partial_x \equiv \partial/\partial x$. The potential density $\omega$ splits into an interfacial, a bulk elastic contribution and a chemical contribution $\omega = \omega_{\text{int}} + \omega_{\text{el}} + \omega_{\text{ch}}$. The continuous fields describing the evolution of the system are the phase-field $\varphi$, which discriminates between the fcc matrix ($\varphi = 0$) and the ordered $\gamma''$ phase ($\varphi = 1$) as well as the elastic displacement field $\{u_i\} = (u_x, u_y, u_z)$, which describes the local distortion of a material point by elastic deformations.

Interfacial contribution

The interfacial contribution to the potential functional is

$$\omega_{\text{int}} = \frac{\Gamma_0}{\Gamma_0} (\partial_i \varphi \partial_i \varphi) + \frac{\Gamma}{\xi \Gamma_0} p(\varphi),$$  \hfill (11)

where a summation over repeated indices is implied. The phase-field parameter $\Gamma$ determines the interface width and the parameter $\Gamma_0$ corresponds to the interfacial energy density. $\Gamma_0$ denotes a calibration factor for the interface energy density, which is calculated via the line integral, $\Gamma_0 = \int \omega_{\text{int}} (\varphi_0, \{\partial_i \varphi_0\}) \, d\Gamma$, where $n$ denotes the direction normal to the interface, and $\varphi_0$ is a phase-field with just one full transition from $\varphi = 0$ to $\varphi = 1$. Further, the equilibrium potential is

$$p(\varphi) = \frac{\xi^2}{\Delta x^2} \left\{ \varphi (1 - \varphi) + \frac{1 - a^2}{4a^2} \log \left( \frac{1 - a^2}{1 - a^2 (1 - 2\varphi)} \right) \right\},$$  \hfill (12)

where the parameter $a = \tanh (2\Delta x/\xi)$ couples to the discretization grid via the numerical grid spacing $\Delta x$. This potential has two local minima at $\varphi = 0$ and $\varphi = 1$, which correspond to the two distinct phases of the system. In the continuum limit $\Delta x \to 0$, this potential converges to the usual quartic double-well potential $p_{\text{const}}(\varphi) = 8\varphi^2 (1 - \varphi)^2$, as $\lim_{\Delta x \to 0} \xi^2 a^2/\Delta x^2 = 4$.

Figure 3 shows the equilibrium potential for $\xi/\Delta x = 2$, which will be used throughout this work as well as for the continuum limit $\xi/\Delta x \to \infty$. The reason for choosing this potential is to diminish effects from the
The phase dependent elastic constants $\tilde{C}_{ij}$ as well as the eigenstrains $\tilde{\varepsilon}_{0,i}$ are interpolated as

$$
\tilde{C}_{ij}(\varphi) = \sum_\alpha \varepsilon(\varphi)C_{ij}^\alpha \tag{15}
$$
$$
\tilde{\varepsilon}_{0,i}(\varphi) = \sum_\alpha h(\varphi)\varepsilon_{0,i}^\alpha, \tag{16}
$$

where $\alpha$ denotes the considered phase and $\varphi$ denotes the local phase-field parameter. We interpolate on the level of the elastic parameters, not on the level of the bulk energies to minimize the amount of interfacial excess energy $[72]$. A Lagrangian formulation in the small strain approximation is used. The local stress tensor is defined as the partial derivative of the elastic energy density Equation (14) with respect to the strain tensor,

$$
\sigma = \frac{\partial \omega_{el}}{\partial \varepsilon}. \tag{17}
$$

The solution for the elastic displacement field is given by the condition of mechanic equilibrium

$$
\frac{\delta \Omega}{\delta u_i} = \frac{\partial}{\partial x_i} \frac{\partial \omega_{el}}{\partial \varepsilon} = \frac{\partial \sigma}{\partial x_i} = 0, \tag{18}
$$

In summary, the model requires to solve the full set of coupled partial differential equations of second order, as given by Equation (13) for the phase-field and Equation (18) for the elastic displacements. With regard to the mechanical equilibrium, that is assumed at every time step of the phase-field solver, we perform a Jacobi relaxation.

### Chemical contribution

Realistic microstructure exhibit conserved phase volumes, due to the conservation of mass $[55]$. Here, the preserved phase volume is achieved by the chemical contribution to the potential energy density

$$\omega_{ch}(t) = h(\varphi)f_{ch}(t), \tag{19}$$

which contains an extra time-dependent and homogeneous driving force contribution $f_{ch}(t)$, such that a volume change of the precipitate phase is prohibited $[73]$. A more sophisticated description of the kinetics of diffusion-limited precipitation, which explicitly involves the chemical diffusion of multiple alloying elements, is also possible $[55, 67]$, but beyond the scope of the present work.

The phase fraction $V_\alpha$ is conserved when

$$0 = \frac{d}{dt} V_\alpha(t) = \int_V \frac{\partial}{\partial t} \varphi(x,t)dV. \tag{20}$$

Inserting the right-hand side of phase-field Equation (13) into (20), we obtain the time-dependent homogeneous driving force

$$f_{ch}(t) = \frac{3G \xi}{2H(t)}. \tag{21}$$

### Elastic contribution

The elastic contribution to the potential energy density $\omega_{el}$ is defined in terms of the phase-dependent elastic properties: the total strain field $\varepsilon$ that is derived from the local displacements $u_i$, the misfit strain $\tilde{\varepsilon}_0$ of the precipitate phase, and the phase-dependent elastic constants $C$ $[55]$. Specifically the elastic energy density is written as

$$\omega_{el}(\varphi,x) = \frac{1}{2}(\varepsilon - \tilde{\varepsilon}_0)\tilde{C}(\varepsilon - \tilde{\varepsilon}_0). \tag{14}$$

In conjunction with the formulation of the interfacial contribution, we impose an interpolation function $h(\varphi) = \varphi^2(3 - 2\varphi)$ for any elastic and chemical energy density contribution: $\omega_{el} + \omega_{ch} = \omega_{el}(h(\varphi)) + \omega_{ch}(h(\varphi))$. This is the minimal polynomial satisfying the necessary interpolation conditions $h(0) = 0$ and $h(1) = 1$ and also having a vanishing slope at $\varphi = 0$ and $\varphi = 1$, to not shift the bulk states in the presence of finite driving forces $[70, 71]$. The Allen Cahn-type phase-field evolution equation is

$$\frac{\partial \varphi}{\partial t} = \frac{-2M \delta \Omega}{3T \xi \delta \varphi} + \frac{2M}{3T \xi} \left( \frac{\partial \omega}{\partial \varphi} - \omega \frac{\partial \omega}{\partial \varphi} \right)$$

$$= M \left( \frac{2}{3T_\alpha} \left( \frac{\partial \omega}{\partial \varphi} - \frac{1}{\xi^2} \frac{\partial \varphi}{\partial \varphi} \right) - \frac{2}{3T \xi} \frac{\partial h}{\partial \varphi} \right), \tag{13}
$$

where $M$ is the interface mobility that is chosen as high as possible while still guaranteeing stability of the solver. All these equations are solved by finite difference schemes operating on one fixed square grid with an explicit Euler-type time integration.

### Elastic contribution

Figure 3. Plot of the equilibrium potential given in Equation (3) as a function of the phase-field variable $\varphi$ for different values of $\xi/\Delta x$.

The solution for the elastic displacement field is given by the condition of mechanic equilibrium

$$\frac{\delta \Omega}{\delta u_i} = \frac{\partial}{\partial x_i} \frac{\partial \omega_{el}}{\partial \varepsilon} = \frac{\partial \sigma}{\partial x_i} = 0, \tag{18}$$

In summary, the model requires to solve the full set of coupled partial differential equations of second order, as given by Equation (13) for the phase-field and Equation (18) for the elastic displacements. With regard to the mechanical equilibrium, that is assumed at every time step of the phase-field solver, we perform a Jacobi relaxation.
where the following abbreviations are introduced:

$$G(t) = \int_V \left( \partial_t (\partial_t \varphi) - \frac{8}{\xi^2} \partial_t \varphi \right) dV, \quad (22)$$

$$H(t) = \int_V \frac{\partial h}{\partial \varphi} dV. \quad (23)$$

This method for achieving preserved phase volumes can also be applied to configurations involving more than two phases [74].

**Boundary conditions**

All simulations are carried out in rectangular two-dimensional domains. Elastic interactions between neighboring precipitates can be adjusted by changing the domain size with respect to the size of the initial precipitate. For both cubic and tetragonal symmetry, it is sufficient to model one quarter of the particle with respective mirror boundary conditions. Therefore, for every considered spatial dimension exists one mirror boundary and one opposing domain boundary that ensures periodicity (henceforth referred to as the periodic boundary). The phase-field is imposed with no-flux boundary conditions in both cases.

For the elastic displacement fields, standard boundary conditions such as periodic conditions, strain-free conditions or stress-free boundary conditions are not useful. Here, a distinction is required due to the following reasons. If simple stress-free condition are imposed the state of deformation turns non-uniform, and the boundary loses its flatness, which conflicts with the periodicity of the system. Periodic or strain-free conditions conserve periodicity, but do not allow for the misfitting precipitate to change the volume of the simulation domain and/or its aspect ratio, leading to unrealistically high total deformation energies.

Therefore, at the mirror boundaries vanishing normal displacements \( u_n = 0 \) and vanishing shear strains \( \partial u_n / \partial n = 0 \) are imposed, where \( u \) denotes the elastic displacement field, \( n \) and \( t \) denote the direction normal and tangential to the boundary, respectively. At the opposing periodic boundary again vanishing shear strain conditions are imposed. But for the normal displacement, we homogeneously impose \( u_n = \bar{u}_n \), where \( \bar{u}_n \) denotes the average value of all normal displacements at the boundary. Homogeneous normal displacements are required to avoid conflicts with the periodicity of the systems and to not introduce strain artifacts. The average overall normal displacements at the boundary is used to allow for the volume change, which leads to more realistic total deformation energies. This boundary condition has previously been applied to finite-element modeling of misfit stresses [75–78] and equilibrium shapes [23] in the \( \gamma' \) system. Due to these boundary conditions, all opposing domain boundaries stay parallel yet no spurious elastic energy is introduced through artificial volume conservation.

Figure 4a) shows a simulation domain with an aspect ratio of 2.5 and the imposed boundary conditions for the displacements normal to the boundaries. Modeling a precipitate in a periodic configuration implies an arrangement of the precipitates in a strict long-range order. Specifically, the above boundary conditions imply a superstructure in which the precipitates are arranged in the corners of a cuboidal unit-cell [23] with the distance to each nearest neighbor being twice the domain side lengths. Henceforth this configuration will be referred to as a rectangular superstructure.

By application of antisymmetric variation boundary conditions at one periodic boundary, one can change the arrangement superstructure [79]. Therefore the tangential strains and the phase-field must be imposed with a point-symmetric operation with respect to a bisecting point of the respective domain boundary. Figure 4b) shows the rectangular superstructure and Figure 4c) and d) show two hexagonal arrangements henceforth referred to as hexagonal\(_x\) and hexagonal\(_y\). The respective bisecting point that is used for the antisymmetry operation is indicated as a red dot. Antisymmetric boundary conditions applied to more than one boundary lead to virtual simulation domains that include more than one precipitate. This state is not represented by the actual simulation domain and renders non-physical solutions.

**SIMULATION RESULTS AND DISCUSSION**

To determine the shape of coherent \( \gamma'' \) precipitates we set up phase-field simulations considering the interfacial energy and elastic contributions with constant \( \gamma'' \) phase fraction. Beginning from an arbitrary precipitate shape the phase-field converges towards the minimum of the total energy. The lower left edge of the domain lies in the precipitates center point with the domain boundaries being parallel to the crystallographic [100] and [001] directions. The observed phase fraction in two dimensions appears higher than the respective three-dimensional phase fraction. Beginning from the discussed initial simulation configuration the system was relaxed for a minimum of \( 4 \cdot 10^5 \) iterations. Subsequently the aspect ratio and the total energy contributions were evaluated.

To describe the ratio between interfacial and elastic contribution to the pattern formation we introduce a dimensionless parameter \( L \) similar to the one presented in [18] as

$$L = \frac{l C_{44} \varepsilon_3^2}{\Gamma}, \quad (24)$$

where \( C_{44} \varepsilon_3^2 \) is the elastic energy density scale with the shear modulus \( C_{44} \) of the homogeneous isotropic elastic
\[ \varphi = 1 \]
\[ \varphi = 0 \]

simulation domain
aspect ratio = 2.5

mirror boundary \[ u_i^n = 0 \]

periodic condition \[ u_i^n = \bar{u}_n \]

\[ \text{[100]} \]
\[ \text{[001]} \]

[001] hexagonal \( x \)

[100] hexagonal \( y \)

data provided in Table II and the largest misfit strain \( \varepsilon_3 \) from Table III to make it independent of the misfit ratio \( \varepsilon_3/\varepsilon_1 \). \( \Gamma \) is the isotropic interfacial energy density. The length scale of a particle is defined as \( l = \sqrt{Rr} \) and will be used to normalize lengths. \( R \) denotes the major half axes and \( r \) the minor half axis of the precipitate, as shown in Figure 2 on page 2.

**Variation of anisotropic misfit and elastic constants**

To evaluate the influence of the anisotropy of the misfit strains given in Table III, the simulation domain was chosen to be \( 50 \times 50 \) gridpoints with one quarter of an initial, spherical particle with a 10 gridpoint radius in the bottom left corner. The low phase content together with homogeneous and isotropic elastic material data leaves only the misfit ratio \( \varepsilon_3/\varepsilon_1 \) and the interfacial energy density \( \Gamma \) to determine the equilibrium shape. In this configuration the tetragonal symmetry of the misfit strain is the cause of the plate shape of the \( \gamma'' \) precipitates. There is significant uncertainty about the absolute values of the lattice misfit strain \( \varepsilon_1 \) (see Table III). The misfit strain \( \varepsilon_3 \) is fixed to a value of \( 30 \cdot 10^{-3} \) and \( \varepsilon_3/\varepsilon_1 \) is varied to examine the influence of the anisotropy of the misfit strain on the precipitate shape.

Figure 5a) shows the precipitate aspect ratio as determined by the phase-field model as a function of the misfit ratio \( \varepsilon_3/\varepsilon_1 \). At \( \varepsilon_3/\varepsilon_1 = 1 \) the precipitates are circular with an aspect ratio of 1. With rising misfit ratio the precipitates show elliptical shapes with an aspect ratio that rises until a plateau is reached. In the plateau region, changes in the misfit ratio do no longer influence the precipitate shape. For all considered values of \( L \) the plateau is reached at \( \varepsilon_3/\varepsilon_1 \geq 3 \). The misfit data considered in Table III lies between \( \varepsilon_3/\varepsilon_1 = 6 \) and 60 and thus lies inside the plateau region.

In Figure 5a) the simulations are compared to an analytical model for the optimum shape of \( \gamma'' \) precipitates. The phase-field model as a function of the misfit ratio \( \varepsilon_3/\varepsilon_1 \) and the periodic boundary conditions that allow for volume change of the domain are indicated by solid red lines, respectively. b) The implied rectangular precipitate superstructure. c) and d) Precipitate arrangements hexagonal \( x \) and hexagonal \( y \) that arise from point symmetry centers indicated by a red dot.

Figure 5a) shows the precipitate aspect ratio as determined by the phase-field model as a function of the misfit ratio \( \varepsilon_3/\varepsilon_1 \). At \( \varepsilon_3/\varepsilon_1 = 1 \) the precipitates are circular with an aspect ratio of 1. With rising misfit ratio the precipitates show elliptical shapes with an aspect ratio that rises until a plateau is reached. In the plateau region, changes in the misfit ratio do no longer influence the precipitate shape. For all considered values of \( L \) the plateau is reached at \( \varepsilon_3/\varepsilon_1 \geq 3 \). The misfit data considered in Table III lies between \( \varepsilon_3/\varepsilon_1 = 6 \) and 60 and thus lies inside the plateau region.

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Figure 5. a) Precipitate aspect ratio as a function of the misfit ratio $\varepsilon_3/\varepsilon_1$ for three different $L$ considering homogeneous and isotropic elasticity without elastic interaction with neighboring precipitates. The range in which realistic values for $\gamma''$ lie is indicated in gray (see Table III). Symbols are phase-field results and the lines are taken from the model given in Equation (25) and (26). b) Polar plots of the elastic energy function $B(\vec{n})$ for different orientations of the interface normal $\vec{n}$ in the (010) plane and different misfit ratios $\varepsilon_3/\varepsilon_1$.

Figure 6 shows the aspect ratio of the precipitates as a function of $L$ for a realistic misfit ratio $\varepsilon_3/\varepsilon_1 = 60$. The aspect ratios of the plate-shaped precipitates increase with increasing $L$ as the elastic bulk energy of the system dominates the interfacial part. The precipitate shapes were found to be ellipses with aspect ratios close to the prediction of Equation (25) and (26). The good agreement between the two-dimensional phase-field model and the three-dimensional analytical model in Figure 5a) and 6 suggests that a two-dimensional model is sufficient to describe the aspect ratio of a $\gamma''$ precipitate.
Figure 7a) shows the influence of inhomogeneous elastic properties for precipitate and matrix phase on the precipitate shape as well as the influence of anisotropy of the elastic constants (see Table II). The simulation configuration is the same as in Figure 5a) with $\varepsilon_3/\varepsilon_1 = 60$ and $L = 4$. For reference, the circular shape of a precipitate with an isotropic misfit ($\varepsilon_1 = \varepsilon_3 = 30 \cdot 10^{-5}$) and isotropic homogeneous elasticity is given. In the considered case inhomogeneous elastic properties do not influence the precipitate shapes significantly. Anisotropic elastic properties lead to an elliptical precipitate with a reduced aspect ratio.

Figure 7b) shows the elastic energy density $B_{\langle ii \rangle}$ (see Equation (27)) for isotropic and tetragonally anisotropic elastic constants (see Table II) and $\varepsilon_3/\varepsilon_1 = 60$. The tetragonal anisotropy of the $\gamma''$ phase leads to the $[100]$ direction being elastically softer than in the isotropic case. For tilted directions orientations $\langle 10h \rangle$ $B$ changes non-uniformly. The ratio of $B_{\langle 100 \rangle}/B_{\langle 001 \rangle}$ does not change significantly compared to the ratio $B_{\langle 100 \rangle}/B_{\langle 10b \rangle}$ with $h \neq \{0, 1\}$. This qualitative change in the energetics of tilted interfaces leads to the observed shortening of the precipitate when anisotropy of the elastic properties is considered.

We conclude that without elastic interaction the formation of plate-shaped $\gamma''$ precipitate shapes is mainly driven by the tetragonally anisotropic misfit in the system. The aspect ratio of the precipitates depends on the misfit strains and on the interfacial energy density. For realistically high misfit ratios $\varepsilon_3/\varepsilon_1 \gg 1$ no influence of the absolute value of $\varepsilon_1$ on the precipitate shape is found. Inhomogeneity of the elastic constants has negligible influence on the precipitate shapes. Anisotropic elastic properties lead to elliptical precipitates with decreased aspect ratios.

**Precipitate superstructure and particle-particle interaction**

A square simulation domain at realistically high phase contents eventually leads to precipitates coagulating. Rectangular simulation domains have to be set up to avoid that. The aspect ratio of the rectangular simulation domains will be discussed as part of the simulation configuration. In the following simulations elastic data of the phases is anisotropic, $L = 4$ and $\varepsilon_3/\varepsilon_1 = 60$ (see Table II and III). We describe the interaction between neighboring precipitates by the particle distance. It is defined as the distance between the centers of the precipitates in $[001]$ or $y$-direction or two times the height of the simulation domain.

Figure 8 shows the results of a simulation study in a domain with a fixed aspect ratio of 2.5 and rectangular superstructure. The size of the initial elliptical precipitate was kept constant ($R = 100$ and $r = 34$ gridpoints) and the relative size of the simulation domain was varied in order to model different particle distances. The aspect ratio of a particle increases by $35\%$ in a system when the particle distance is reduced from $3.8l$ to $1.6l$. Note that due to the conserved aspect ratio of the domain also the particle distance in $x$-direction is reduced simultaneously and the phase fraction is rising. Interestingly, the increase in the aspect ratio at high phase contents does not lead to a simple stretching of the particle but also to a deviation from the elliptical shape. The precipitate shape has reduced curvature along its major extent. Similar elastic interactions affecting the precipitate shape have been reported for $\gamma/\gamma'$ with volume fractions up to $75\%$ [23]. Distant precipitates experience attraction and close precipitates are repulsed leading to an equilibrium matrix channel width between the precipitates [44, 83–85].

Figure 9 shows precipitate shapes influenced by elastic particle-particle interaction in different superstructures at a particle distance of $1.8l$. The determined precipitate shapes subject to different implicit superstructures illustrate the significant influence of long-range order on precipitate shapes. The area of all three shapes is equal. The shapes for rectangular and hexagonal$_x$ arrangement can be approximated with ellipses. The superstructure hexagonal$_x$ shortens the precipitate by $10\%$ but it remains an ellipse. The hexagonal$_x$ arrangement leads to deviation from the elliptical shape visible due to the fact that the phase boundary of the precipitate “rectangular” is intersected twice by the phase boundary of “hexagonal$_x$”. The sites of the intersections are indicated by arrows.

Figure 10 shows the total energy density plotted against the domain aspect ratio for the three possible superstructures at a particle distance of $1.8l$. The hexagonal$_x$ arrangement is the energetically most favorable. The rectangular arrangement is intermediate and the hexagonal$_y$ superstructure shows the highest energy density. The rectangular and the hexagonal$_y$ superstructure both exhibit a steadily dropping energy density for aspect ratios of the simulation domain close to 1. It is only in the energetically most favorable hexagonal$_x$ arrangement that one finds a distinct minimum at an aspect ratio of the simulation domain of $1.8$. The implied microstructure of such an energetically optimum configuration is also given in Figure 10. For spherical precipitates with an isotropic misfit a cubic arrangement was found to be the energetic optimum [16].

The configuration that was found to be the energetically most favorable is the one where precipitates exhibit the largest distance to their nearest neighbors in the direction of the highest misfit strain $\varepsilon_3$. An effect of the high elastic energy contribution in the hexagonal$_y$ arrangement is visible in Figure 9, where it leads to additional shortening of the precipitate. Being the energetically minimum configuration of the presented model
Figure 7. a) Influence of inhomogeneity and anisotropy of the elastic properties on precipitate shapes at \( L = 4 \). Elastic constants are given in Table II. For reference, the circular shape of a precipitate with \( \varepsilon_1 = \varepsilon_3 = 30 \cdot 10^{-3} \) and isotropic homogeneous elasticity is shown. b) Polar plots of the orientation dependent elastic energy function \( B(\vec{n}) \) in the (010) plane for isotropic and tetragonal elastic constants \( \varepsilon_3/\varepsilon_1 \).

Figure 8. Dependence of the precipitate aspect ratio on the particle distance in \( y \)-direction with exemplary precipitate shapes. The aspect ratio of the simulation domain is 2.5. With increasing \( \gamma'' \) volume content, the aspect ratio increases and the precipitates deviate from their elliptical shape.

Figure 9. Equilibrium shapes of precipitates subject to different boundary conditions implying three superstructures. The superstructure nomenclature is introduced in Figure 4. Arrows indicate intersections of the elliptical shape outline (rectangular) with the non-elliptical shape (hexagonal). Approximate the volume fraction as the ratio between the volume of a spheroid with the same aspect ratio as the two-dimensional shape and the volume of a respective three-dimensional simulation domain by exploiting the system’s four-fold rotational symmetry around the tetragonal axis. The approximated volume content \( \tilde{V} \) is then given by

\[
\tilde{V} = \frac{4\pi}{3Ad^3\sqrt{1.8}},
\]

where \( A \) is the aspect ratio of the precipitate and \( d \) is the particle distance normalized by \( l \). As shown in Figure 9 the precipitate shapes deviate from the elliptical shape and therefore assuming a spheroidal precipitate as in Equation (28) is not accurate. We assume that this inaccuracy is negligible as the inaccuracy of the volume content measurement itself is comparably large. Note that the single-variant microstructure discussed in this work reflects material aged under load for several hours.

Energy density of the \( \gamma/\gamma'' \) interface

To reproduce experimentally observed aspect ratios of \( \gamma'' \) precipitates, we set up a simulation study assuming constant misfit strains and isotropic interfacial energy density. The simulation domain has an aspect ratio of 1.8, the initial particle has a radius of 20 gridpoints and a hexagonal\(_h\) superstructure was used. The sizes of the respective simulation domains were set such that they resemble a realistic \( \gamma'' \) volume fraction of 12%. We approximate the volume fraction as the ratio between the volume of a spheroid with the same aspect ratio as the two-dimensional shape and the volume of a respective three-dimensional simulation domain by exploiting the system’s four-fold rotational symmetry around the tetragonal axis. The approximated volume content \( \tilde{V} \) is then given by

\[
\tilde{V} = \frac{4\pi}{3Ad^3\sqrt{1.8}},
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where \( A \) is the aspect ratio of the precipitate and \( d \) is the particle distance normalized by \( l \). As shown in Figure 9 the precipitate shapes deviate from the elliptical shape and therefore assuming a spheroidal precipitate as in Equation (28) is not accurate. We assume that this inaccuracy is negligible as the inaccuracy of the volume content measurement itself is comparably large. Note that the single-variant microstructure discussed in this work reflects material aged under load for several hours.
Figure 10. Mean energy densities of systems plotted against the domain aspect ratio. Results are shown for a particle distance of 1.8l and three different superstructures each. The superstructure nomenclature is introduced in Figure 4. The energetically most favorable microstructure is plotted.

[38, 86] or specifically tailored material [14]. We assume that particle interactions of perpendicularly oriented precipitates lead to the same stretching of the precipitates but might impose further constraint to the growth of precipitates that is not reflected by the proposed model.

Figure 11a) shows experimental data from various sources reporting the aspect ratio of $\gamma''$ precipitates as a function of the precipitate major radius [25, 49, 87, 88]. Interfacial dislocations occur when full coherency of precipitates larger than $R = 25$ nm is lost [25, 48, 49]. Here, we restrict to fully coherent precipitates, as interfacial dislocations alter the strain field around a precipitate [39] in a way that is not reflected by the model. The aspect ratio of the precipitates increase with increasing precipitate size due to the rising importance of elastic bulk effects over the interfacial energy with $L \sim l$ (see Equation (24)). In simulations with a particle distance of 5l an interfacial energy density of 65 mJ m$^{-2}$ to 130 mJ m$^{-2}$ is necessary to reproduce experimentally observed aspect ratios. This is in good accordance with the previously reported isotropic $\gamma''$ interfacial energy density of 95 $\pm$ 17 mJ m$^{-2}$ [25]. This value was obtained by the application of an analytical model for the equilibrium aspect ratio of a $\gamma''$ precipitate given in Equation (25) and (26) based on Eshelby’s inclusion theory [48, 80]. This model assumes isotropic and homogeneous elasticity, isotropic interfacial energy density, a spheroidal precipitate shape and no elastic interaction. The prediction of this model for the size dependent aspect ratio of a precipitate with an interfacial energy density of 90 mJm$^{-2}$ is also shown in Figure 11a). An interfacial energy density of 145 mJm$^{-2}$ was found for D0$_{22}$ precipitates in a Fe-Ni-Ta alloy [48].

Figure 11a) shows that at a realistic volume fraction of 12% the isotropic energy density needed to reproduce experimental findings lies between 90 mJm$^{-2}$ and 200 mJm$^{-2}$, which corresponds to $0.8 < L < 5.4$. In a real system the interfacial energy of a tetragonal to cubic interface might be strongly anisotropic [89, 90], which could also be included in a phase-field model. As to the best of our knowledge, no information about the magnitude of such an anisotropy for the coherent $\gamma''$-interface is available, we assume an isotropic $\Gamma$. The obtained isotropic interfacial energy densities are a factor of 1.5 higher than those determined without consideration of elastic particle-particle interaction. Figure 11a) includes data from averaged aspect ratios generated from TEM images as for example given in Figure 1b). 72 fully coherent $\gamma''$ precipitates in IN718M were evaluated by image analysis. The samples were homogenized at 1423 K for 2 h and subsequently water quenched. The error bar shows the standard deviation of the aspect ratio. For this system, we predict an isotropic interfacial energy density of 220 mJ m$^{-2}$.

Figure 11b) illustrates the influence of the competing factors discussed above on the aspect ratio of a precipitate. A higher the interfacial energy density $\Gamma$ provides a tendency towards more spherical precipitates, i.e. smaller aspect ratios. Stronger elastic interactions between precipitates at higher volume fraction $V$, in turn, lead to higher precipitate aspect ratios (see Figure 11a). To estimate the interfacial energy density from the experimentally observed aspect ratios of precipitates it is crucial to take into account the elastic interactions of precipitates at finite volume fractions.

Comparison of theoretically determined equilibrium shapes with experimentally observed shapes is a possible way to get information about the interfacial energy [24–26]. However, the accuracy of this method is limited by the underlying model description of the equilibrium shape and by the possibility to experimentally observe precipitates in their equilibrium. The model presented in this work is in many ways an improvement over existing analytical models as it takes into account elastic interactions between precipitates in a two-dimensional optimum, non-rectangular arrangement and tetragonal/cubic anisotropy of the elastic constants for both phases. It is limited by being only a realistic description of a uniform single-variant microstructure that does not take into account the kinetics of precipitate growth that might have strong influence on the shapes of experimentally observed precipitates [91]. It was also found that a periodic arrangement of precipitates must not always be a stable configuration [46].

**CONCLUSION**

We evaluate influencing factors on equilibrium shapes of $\gamma''$ precipitates in Ni-based superalloys considering one
Figure 11. a) Data set of precipitate aspect ratio over major radius in the regime of fully coherent interfaces [25, 49, 87, 88]. Simulation-based estimates for a lower and upper boundary of the interfacial energy density are given for a γ'' volume fraction of 12%. The prediction of the size dependent aspect ratio of γ'' precipitates with an interfacial energy of 90 mJ m$^{-2}$ by the analytical model of Cozar & Pineau is also shown [48]. b) Schematic plot illustrating the competing effects of volume fraction $V$ and interfacial energy density $\Gamma$ on the precipitate aspect ratio.

orientational variant. The shapes are determined using a phase-field formulation taking into account interfacial and elastic energy contributions.

1. At negligible elastic particle-particle interaction, the phase-field model provides elliptic equilibrium shapes γ'' that are fully consistent with former analytic descriptions [48, 80]. The aspect ratio $R/r$ of a precipitate increases with increasing misfit strain $\varepsilon_3$. The precipitate shape is influenced by $\varepsilon_1$ only for $\varepsilon_3/\varepsilon_1 \leq 3$. Inhomogeneity and anisotropy of the elastic constants have less significant influence on the γ'' precipitate shape.

2. Elastic particle-particle interactions significantly influence precipitate shapes at realistically high volume fractions. Different periodic arrangements of γ'' precipitates are modeled by respectively tailored boundary conditions. A decreased particle distance leads to an increased precipitate aspect ratio.

3. Non-volume conserving displacement boundary conditions allow precise determination of the total energy density of periodic precipitation microstructures. The energetically most favorable superstructure is a hexagonal$_x$ precipitate arrangement (see Figure 4c).

4. The evaluation of interfacial energy density based on equilibrium shapes is sensitive to the phase content. At a realistic volume fraction of 12%, an interfacial energy density between 90 and 200 mJ m$^{-2}$ leads to precipitate aspect ratios that match experimental observations. Respective interfacial energy densities determined without accounting for elastic interaction between the precipitates are 30 % lower.

CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

F. Schleifer: Conceptualization, Methodology, Software, Validation, Formal Analysis, Investigation, Writing – Original Draft, Visualization. M. Holzinger: Conceptualization, Methodology, Software. Y.-Y. Lin: Conceptualization, Investigation, Data Curation, Validation. U. Glatzel: Supervision, Resources, Writing – Review & Editing, Project Administration, Funding Acquisition. M. Fleck: Conceptualization, Software, Supervision, Writing – Review & Editing, Project Administration, Funding Acquisition.

DECLARATION OF COMPETING INTEREST

Authors have no conflict of interest to declare.

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