Introduction

This book[1,2] presents original mathematical models of

- thermal and phase-transformation stresses, which originate during a cooling process in model material systems, i.e., multi-particle-envelope-matrix and multi-particle-matrix systems, corresponding to real three- and two-component materials (see Chapters 2–4), respectively,

- intercrystalline and transcrystalline crack formation in components of these model material systems, including mathematical definitions of critical limit states with respect to the material crack formation, which is induced by these stresses (see Chapter 5).

- material micro- and macro-strengthening in components of these model systems, which is induced by these stresses (see Chapter 6).

The material strengthening and the limit states represent important phenomena in material science and engineering. The multi-particle-envelope-matrix and multi-particle-matrix model systems consist of isotropic spherical particles with and without an isotropic spherical envelope on the particle surface, which are periodically distributed in an isotropic matrix (see Section 1.1). The interparticle distance d, the particle radius R_1, the envelope radii R_1, R_2 and the particle volume fraction v_p represent parameters of these model systems, as well as microstructural parameters of three- and two-component materials.

The multi-particle-envelope-matrix system corresponds to real three-component materials (see Section 1.1), which consist of

[1] This book was reviewed by the following reviewers:
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- isotropic precipitates with an isotropic continuous component on their surfaces, distributed in isotropic crystalline grains, e.g., matrix-precipitate-envelope composites,

- isotropic crystalline grains with and without an isotropic continuous component (E) on their surfaces, and the crystalline grains exhibit identical or different material properties, i.e., the real three-component material consists of the crystalline grains $A+E$, A or $A+E$, B, respectively, where A, B represent crystalline grains with different material properties.

The multi-particle-matrix system corresponds to real two-component materials, which consist of

- isotropic precipitates, distributed in isotropic crystalline grains, e.g., matrix-precipitate composites,

- two types of isotropic crystalline grains with different material properties, e.g., dual-phase steel with the grains A and B.

The relationships between the model material components and those of the real three- and two-component materials are determined in Section 1.1.

The thermal stresses are a consequence of different thermal expansion coefficients of the matrix, the envelope and the particle. The phase-transformation stresses are a consequence of a different dimension of a cubic crystalline lattice (see Section 1.3), which is transformed in the material component. Mathematical and computational models of phenomena in infinite periodic model material systems are determined within identical suitable cells, and each cell contains a central component with or without the envelope. Due to this infinity and periodicity, the mathematical and computational models, which are determined for a certain cell, are valid for any cell. Infinite matrixes are used due to simplicity of mathematical solutions for material components (e.g., precipitates, pores). The material components are small in comparison with macroscopic material samples or macroscopic structural elements, and then the solutions are acceptable in spite of this simplification [1]. The mathematical models results from fundamental equations of mechanics of a solid continuum, with respect to its shape, loading, mechanical constraints and the principle of minimum potential energy.

Additionally, the stress fields, i.e., the thermal and phase-transformation stresses, in neighbouring cells are mutually affected. The stress field in a certain cell is then affected by those in neighbouring cells, and vice versa. In contrast

to [2, 3], this effect is explicitly determnined by the superposition method of mechanics of a solid continuum (see Section 1.8.3) [4, 5].

The infinite multi-particle-envelope-matrix and multi-particle-matrix systems are imaginarily divided into cubic cells with the dimension *d* and with a central spherical particle with or without the spherical envelope on the particle surface, and the stresses are determined within the cubic cell (see Section 1.1). Mathematical solutions for these model systems correspond to real composites, in contrast to

- the simple one-particle mathematical model in [6], which is determined for a simple one-particle-matrix model system,
- the simple multi-particle mathematical model in [7], which is determined for physically unacceptable mechanical constraints due to unsuitable cells of a multi-paticle-matrix system.

Different mathematical procedures, which are applied to the fundamental equations (i.e., Cauchy's and equilibrium equations, Hooke's law), determined with respect to a suitable ccordinate system (see Sections 1.2, 1.5), result in different mathematical solutions for the stresses in the matrix, the envelope and the particle (see Sections 1.6, 2.1, 3.1, 4.1). Finally, such a combination of the different mathematical solutions for these components is considered to exhibit minimum potential energy (see Section 1.7). The mathematical models are determined by standard procedures of mechanics of a solid continuum, which include definitions of

- such model material systems, which corresponds to real three- and two-component materials (Section 1.1),
- such a coordinate system, which corresponds to geometry of the model systems (Section 1.2),
- reasons of the thermal and phase-transformation stresses (Section 1.3),
- the loading of the model material systems (Section 1.4)
- the fundamental equations, which sre determined with respect to the coordinate system (Section 1.5), and result in a system of differential equations (Section 1.6),
- elastic energy density, elastic energy and total energy of the model material systems (Section 1.7),

- mechanical constraints, i.e., mathematical boundary conditions, for the components of the model material systems (Sections 1.8.1, 1.8.2),
- the superposition method (see Section 1.8.3), which is considered within the mathematical models of the thermal and phase-transformation stresses (see Section 1.8.3),
- different mathematical procedures (see Sections 2.1, 3.1, 4.1), which are applied to the system of the differential equations (Section 1.7),
- final formulae for the thermal and phase-transformation stresses, strains, elastic energy density and elastic energy (see Sections 2.2–2.5, 3.2, 3.3, 4.2, 4.3),
- mathematical procedures to determine
  - such critical radii of the spherical envelope and the spherical particle, which are reasons of cracks in the components of the model material systems,
  - shapes and dimensions of the component cracks,
- formulae for the micro-strengthening in the material components, along with formulae for the macro-strengthening in the cubic cell, i.e., in the multi-particle-envelope-matrix and multi-particle-matrix systems.

The mathematical results in this monograph are then applicable within

- basic research (mechanics of a solid continuum, theoretical physics, material science),
- the engineering practice, i.e., material technology,
- as well as within university undergraduate and postgraduate courses, as a textbook on analytical material mechanics.

With regard to the basic research, the results of this monograph can be incorporated to mathematical models, which defines the disturbance of an applied stress field around inclusions in a solid continuum [8], as well as into mathematical, computational and experi-mental models of overall materials stresses, overall material strengthening, interactions of energy barriers with dislocations and domain walls, etc. The mathematical models include parameters of the multi-particle-envelope-matrix and multi-particle-matrix system, i.e., v_p,

d, R_1, R_2, which represent microstructural parameters of real three- and two-component composites, respectively. In case of real three- and two-component composites, (the engineering practice), material scientists and engineers can determine such numerical values of the microstructural parameters,

- which result in maximum values of the material micro- and macro-strengthening,
- which define the limit states (i.e., critical states) with respect to the intercrystalline or transcrystalline crack formation in the components of the real composites.

In case of homogeneous or heterogeneous microstructure of a real composite material, the microstructural parameters are defined by mean or local numerical values, respectively. Consequently, the material scientists and engineers can develop suitable technological processes, which result in such microstructural parameters to obtain maximum strengthening, and to avoid the crack formation.

This numerical determination, performed by suitable programming languages, result from the mathematical procedure in Appendix. With respect to the university courses, the fundamental equations of mechanics of a solid continuum, along with the mathematical procedures, are explained and determined in detail. As a textbook on analytical material mechanics, this monograph is then suitable for non-specialists in mechanics of a solid continuum. Finally, Appendix presents such mathematical topics, which are required to perform the mathematical procedures in this monograph.

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Chapter 1

Solid Continuum Mechanics

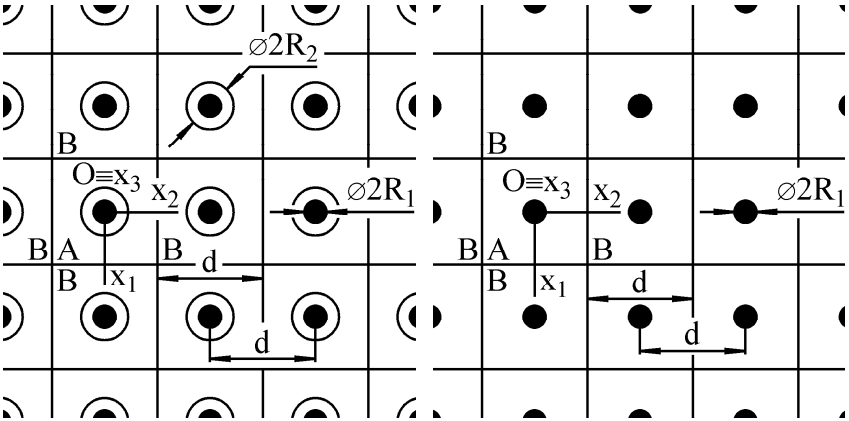
1.1 Model Material System

Figures 1.1a and 1.1b show model material systems, which correspond to real three- and two-component materials [9], i.e., the multi-particle-envelope-matrix and multi-particle-matrix systems, respectively. The multi-particle-envelope-matrix and multi-particle-matrix systems systems consist of isotropic spherical particles with and without an isotropic spherical envelope on their surface, respectively. The spherical particles with or without the spherical envelope are periodically distributed in an isotropic infinite matrix with the interparticle distance d along the axes x_1, x_2, x_3 of the Cartesian system $(Ox_1x_2x_3)$, where the point O is a centre of the spherical particle.

The model material systems are imaginarily divided into identical cubic cells with the centre O and with the dimension d. Each cell contains a central spherical particle with or without the spherical envelope, where R_1 is a radius of the particle, and R_1, R_2 are radii of the envelope. The cubic cell represents such a part of the model material systems, which is related to one spherical particle. The matrix is infinite along the axes x_1, x_2, x_3. The model material systems in Figure 1.1 are depicted in the plane x_1x_2 of the Cartesian system $(Ox_1x_2x_3)$. Due to infinity and periodicity of the model material systems, the same figure is also considered for the planes x_1x_3 and x_2x_3.

As presented in [1], mathematical and computational models of phenomena in infinite periodic model material systems are determined within identical suitable cells. Due to this infinity and periodicity, mathematical and computational results, which are determined for a certain cell, are valid for any cell.

The mathematical models of the thermal and phase-transformation stresses in the spherical particle, the spherical envelope, and the cell matrix for the infinite and periodic model material systems in Figure 1.1 are determined within the cubic cell. Infinite matrixes are used due to simplicity of mathematical solutions for material components (e.g., precipitates, pores, crystalline grains). The material components are small in comparison with macroscopic material samples or macroscopic structural elements, and then the solutions are acceptable in spite of this simplification [1].



(a) (b)

Figure 1.1: (a) The multi-particle-envelope-matrix and (b) the multi-particle–matrix systems are imaginarily divided into identical cubic cells with the dimension d and with a central spherical particle. The spherical particles with and without a spherical envelope on their surface are periodically distributed in the infinite matrix, where R_1 is a radius of the particle, and R_1, R_2 are radii of the envelope. The matrix is infinite along the axes x_1, x_2, x_3 of the Cartesian system $(Ox_1x_2x_3)$, where O is identical with a centre of the spherical particles. The thermal and phase-transformation stresses in the cell A and the neighbouring cells B are mutually affected.

Additionally, the stress fields, i.e., the thermal and phase-transformation stresses, in neighbouring cells are mutually affected. The stress field in the cell A is then affected by those in the neighbouring cells B, and vice versa (see Figure 1.1). In contrast to [2, 3], this effect is explicitly determnined by the superposition method of mechanics of a solid continuum [4, 5].

With regard to the volume $V_p = 4\pi R_1^3/3$ and $V_C = d^3$ of the spherical particle and the cubic cell, respectively, the particle volume fraction v_p and the interparticle distance d have the forms

$$v_p = \frac{V_p}{V_C} = \frac{4\pi}{3}\left(\frac{R_1}{d}\right)^3 \in (0, v_{i\,max}\rangle\,, \quad d = R_1\left(\frac{2\pi}{3v_p}\right)^{1/3}, \quad i = 1,2,$$
$$v_{1\,max} = \frac{\pi}{6}, \quad v_{2\,max} = \frac{\pi}{6}\left(\frac{R_1}{R_2}\right)^3, \tag{1.1}$$

where $v_{1\,max}$ and $v_{2\,max}$ result from the condition $d = 2R_1$ and $d = 2R_2$ for

the multi-particle-matrix and multi-particle-envelope-matrix systems, respectively. Additionally, v_p, d, R_1, R_2 represent fundamental characteristics of real two- and three-component material, which are determined by experimental and computational techniques.

The multi-particle-envelope-matrix system in Figure 1.1a corresponds to real three-component materials, which consist of

- isotropic precipitates with an isotropic continuous component on their surfaces, distributed in isotropic crystalline grains, e.g., matrix-precipitate-envelope composites,

- isotropic crystalline grains with and without an isotropic continuous component (E) on their surfaces, and the crystalline grains exhibit identical or different material properties, i.e., the real three-component material consists of the crystalline grains $A+E$, A or $A+E$, B, respectively, where A, B represent crystalline grains with different material properties.

The precipitates, the continuous component and the crystalline grains are considered to represent the spherical particles, the spherical envelope and the matrix of the multi-particle-envelope-matrix system, respectively.

Similarly, the crystalline grains with the continuous component, the continuous component and the crystalline grains without the continuous component are considered to represent the spherical particles, the spherical envelope and the matrix of the multi-particle-envelope-matrix system, respectively.

The multi-particle-matrix system in Figure 1.1b corresponds to real two-component materials, which consist of

- isotropic precipitates, distributed in isotropic crystalline grains, e.g., matrix-precipitate composites,

- two types of isotropic crystalline grains with different material properties, e.g., dual-phase steel with the grains A and B.

Consequently, the precipitates and the crystalline grains are considered to represent the spherical particles and the matrix of the multi-particle-matrix system, respectively. Similarly, let the crystal grains A and B be characterized by the volume fraction v_A and v_B, respectively, where $v_A + v_B = 1$. If $v_A < v_B$, then the grains A and B are considered to represent the spherical particles and the matrix, respectively. If $v_A > v_B$, then the grains A and B are considered to represent the matrix and the spherical particles, respectively. If $v_A = v_B$, then the following energy analysis is required to be considered. Let the grains A

and B be considered to represent the spherical particles and the matrix with the elastic energy W_{pA} and W_{mB}, which is accumulated in one spherical particle and the cell matrix (see Equations (1.63), (1.64)), respectively. Let the grains A and B be considered to represent the matrix and the spherical particles with the elastic energy W_{mA} and W_{pB}, which is accumulated in the cell matrix and one spherical particle (see Equations (1.63), (1.64)), respectively. If $W_{pA}+W_{mB}<W_{mA}+W_{pB}$, then the grains A and B are considered to represent the spherical particles and the matrix, respectively. If $W_{pA}+W_{mB}>W_{mA}+W_{pB}$, the grains A and B are considered to represent the matrix and the spherical particles, respectively.

1.2 Coordinate System

The thermal and phase-transformation stresses are determined at the arbitrary point P along the axes x_1', x_2', x_3' of the Cartesian system $\left(Px_1'x_2'x_3'\right)$ with the unit vectors $\vec{e}_1{}'$, $\vec{e}_2{}'$, $\vec{e}_3{}'$ (see Figure 1.2), respectively. The point P is defined by the spherical coordinates (r,φ,ν), which are considered due to the spherical particles and spherical envelopes (see Figure 1.1).

The thermal and phase-transformation stresses are determined within the cubic cell. The model material systems in Figure 1.1 are symmetric. Accordingly, the thermal and phase-transformation stresses are sufficient to be determined within one eighth of the cubic cell (see Figure 1.3), i.e., for $\varphi\in\langle 0,\pi/2\rangle$ and $\nu\in\langle 0,\pi/2\rangle$. The intervals $r\in\langle 0,R_1\rangle$, $r\in\langle R_1,R_2\rangle$, and $r\in\langle R_2,r_s\rangle$ are related to the spherical particle, the spherical envelope, and the cell matrix, respectively.

As presented in Figure 1.3, we get $r_s=OS_1$ and $r_s=OS_2$ for $\nu\in\langle 0,\nu^*\rangle$ and $\nu\in\langle\nu^*,\pi/2\rangle$, respectively. The points S_1 and S_2 represent intersections of the axis x_1' with the cell surfaces *3657* and *1456*, respectively. The axis x_1' represents a radial direction (see Figure 1.2), which is defined by the angles $\varphi\in\langle 0,\pi/2\rangle$ and $\nu\in\langle 0,\pi/2\rangle$. The angle ν^* (see Figure 1.3) and the coefficient c_φ are derived as

$$\begin{aligned}
&\nu^*=\arctan\left(\frac{x_{12d}}{\left|\overline{O3}\right|}\right)=\arctan\left(\frac{1}{c_\varphi}\right),\\
&x_{12d}=\left|\overline{O8}\right|=\left|\overline{39}\right|=\frac{d}{2\,c_\varphi},\\
&c_\varphi=\cos\varphi,\quad \varphi\in\left\langle 0,\frac{\pi}{4}\right\rangle,\\
&c_\varphi=\sin\varphi,\quad \varphi\in\left\langle \frac{\pi}{4},\frac{\pi}{2}\right\rangle,
\end{aligned}\tag{1.2}$$