1
Introduction to Crystalline Anisotropy and the Crystal Plasticity Finite Element Method

Crystalline matter is mechanically anisotropic. This means that the instantaneous and time-dependent deformation of crystalline aggregates depends on the direction of the mechanical loads and geometrical constraints imposed. This phenomenon is due to the anisotropy of the elastic tensor, Figure 1.1, and to the orientation dependence of the activation of the crystallographic deformation mechanisms (dislocations, twins, martensitic transformations), Figure 1.2.

An essential consequence of this crystalline anisotropy is that the associated mechanical phenomena such as material strength, shape change, ductility, strain hardening, deformation-induced surface roughening, damage, wear, and abrasion are also orientation-dependent. This is not a trivial statement as it implies that mechanical parameters of crystalline matter are generally tensor-valued quantities. Another major consequence of the single-crystal elastic-plastic anisotropy is that it adds up to produce also macroscopically directional properties when the orientation distribution (crystallographic texture) of the grains in a polycrystal is not random. Figure 1.3a,b shows such an example of a plain carbon steel sheet with a preferred crystal orientation (here high probability for a crystallographic {111} plane being parallel to the sheet surface) after cup drawing. Plastic anisotropy leads to the formation of an uneven rim (referred to as *ears* or *earing*) and a heterogeneous

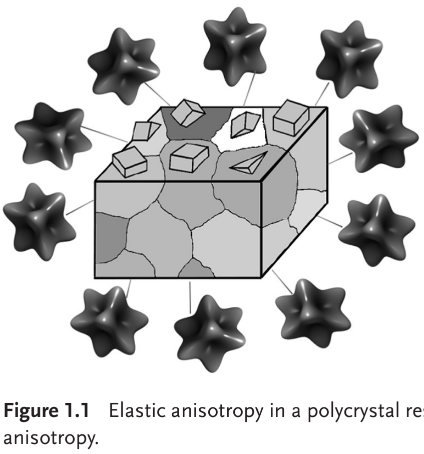

Figure 1.1 Elastic anisotropy in a polycrystal resulting from superposition of single-crystal anisotropy.

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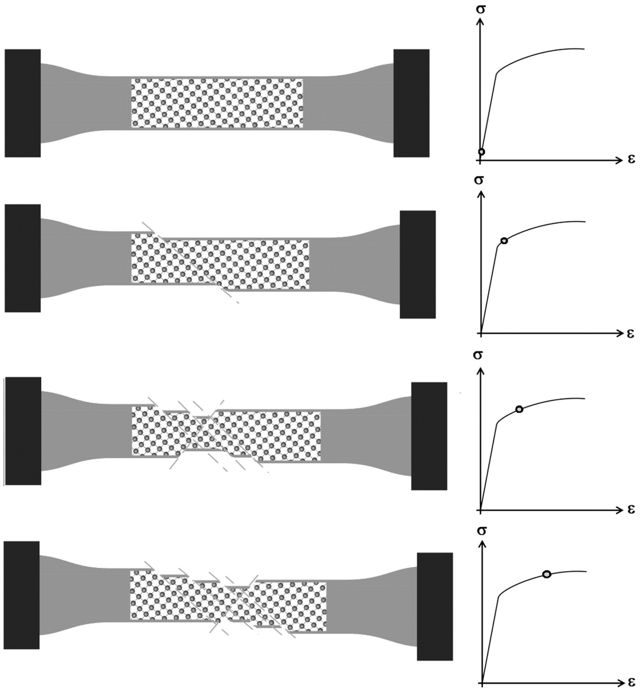
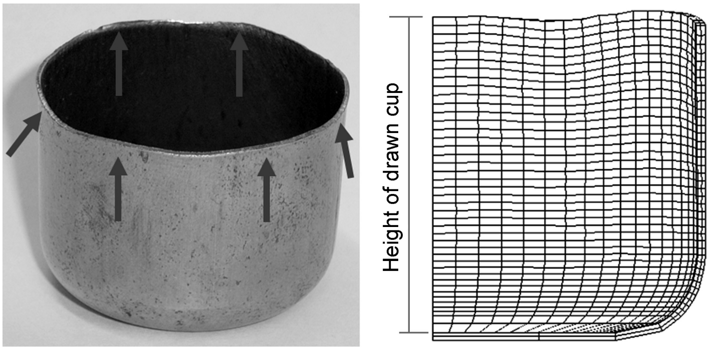


Figure 1.2 Plastic anisotropy in a single crystal due to distinct crystallography.



(a) (b)

Figure 1.3 Consequence of plastic anisotropy when drawing a textured sheet into a cup. The orientation distribution before deformation exhibits a high volume fraction of grains with a crystallographic [111] axis parallel to the sheet normal. The arrows in (a) mark six ears resulting from preferential material flow. (b) The corresponding crystal plasticity finite element simulation.

distribution of material thinning during forming. It must be emphasized in that context that a random texture is not the rule but a rare exception in real materials. In other words, practically all crystalline materials reveal macroscopic anisotropy.

A typical example of such macroscopic anisotropy is the uniaxial stress–strain curve, which is the most important mechanical measure in the design of structural materials. The introductory statement made above implies that uniaxial stress–strain curves represent an incomplete description of plastic deformation as they reduce a six-dimensional yield surface and its change upon loading to a one-dimensional (scalar) yield curve, see Figure 1.4. Another consequence of this statement is that the crystallographic texture (orientation distribution) and its evolution during forming processes is a quantity that is inherently connected with plasticity theory, more precisely, with the anisotropy of the underlying plasticity mechanisms. Texture can, hence, be used to describe the integral anisotropy of polycrystals in terms of the individual tensorial behavior of each grain and the orientation-dependent boundary conditions among the crystals. Formally, the connection between shear and texture evolution becomes clear from the fact that any deformation gradient can be expressed as the combination of its skew-symmetric portion, which represents a pure rotation leading to texture changes if not matched by the rotation implied by plastic shear, and a symmetric tensor that is a measure of pure stretching. Plastic shear, hence, creates both shape and orientation changes, except for certain highly symmetric shears. Therefore, a theory of the mechanical properties of crystals must include, first, the crystallographic and anisotropic nature of those mechanisms that create shear and, second, the orientation(s) of the crys-

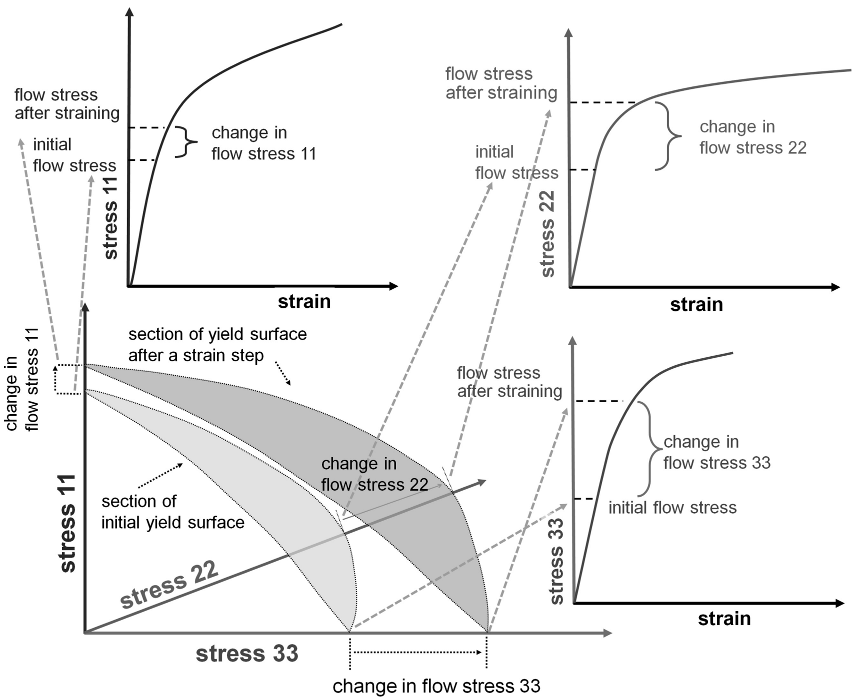


Figure 1.4 Flow stress and strain hardening of anisotropic materials are tensor quantities.

tal(s) studied relative to the boundary conditions applied (e.g., loading axis, rolling plane).

Early approaches to describe anisotropic plasticity under simple boundary conditions considered these aspects, such as the Sachs (1928), Taylor (1938), Bishop–Hill, and Kröner (1961) formulations. However, these approaches were neither designed for considering explicitly the mechanical interactions among the crystals in a polycrystal nor for responding to complex internal or external boundary conditions, see Figure 1.5a–d. Instead, they are built on certain simplifying assumptions of strain or stress homogeneity to cope with the intricate interactions within a polycrystal.

For that reason variational methods in the form of finite element approximations have gained enormous momentum in the field of crystal mechanical modeling. These methods, which are referred to as crystal plasticity finite element (CPFE) models, are based on the variational solution of the equilibrium of the forces and the compatibility of the displacements using a weak form of the principle of virtual work in a given finite-volume element. The entire sample volume under consideration is discretized into such elements. The essential step which renders the deformation kinematics of this approach a crystal plasticity formulation is the fact that the velocity gradient is written in dyadic form. This reflects the tensorial crystallographic nature of the underlying defects that lead to shear and, consequently, to both shape changes (symmetric part) and lattice rotations (skew-symmetric part), see Chapter 3. This means that the CPFE method has evolved as an attempt to employ some of the extensive knowledge gained from experimental and theoretical studies of single-crystal deformation and dislocations to inform the further development of continuum field theories of deformation. The general framework supplied by variational crystal plasticity formulations provides an attractive vehicle for developing a comprehensive theory of plasticity that incorporates existing knowledge of the physics of deformation processes (Arsenlis *et al.*, 2004; Curtin and Miller, 2003; Vitek, Mrovec, and Bassani, 2004a) into the computational tools of continuum mechanics (Zienkiewicz, 1967; Zienkiewicz and Taylor, 2005) with the aim to develop advanced and physically based design methods for engineering applications (Zhao *et al.*, 2004a).

One main advantage of CPFE models lies in their capability to solve crystal mechanical problems under complicated internal and/or external boundary conditions. This aspect is not a mere computational advantage, but it is an inherent part of the physics of crystal mechanics since it enables one to tackle those boundary conditions that are imposed by inter- and intragrain micro-mechanical interactions, Figure 1.6 (Sachtleber, Zhao, and Raabe, 2002). This is not only essential to study in-grain or grain cluster mechanical problems but also to better understand the often quite abrupt mechanical transitions at interfaces (Raabe *et al.*, 2003).

However, the success of CPFE methods is not only built on their efficiency in dealing with complicated boundary conditions. They also offer high flexibility with respect to including various constitutive formulations for plastic flow and hardening at the elementary shear system level. The constitutive flow laws that were

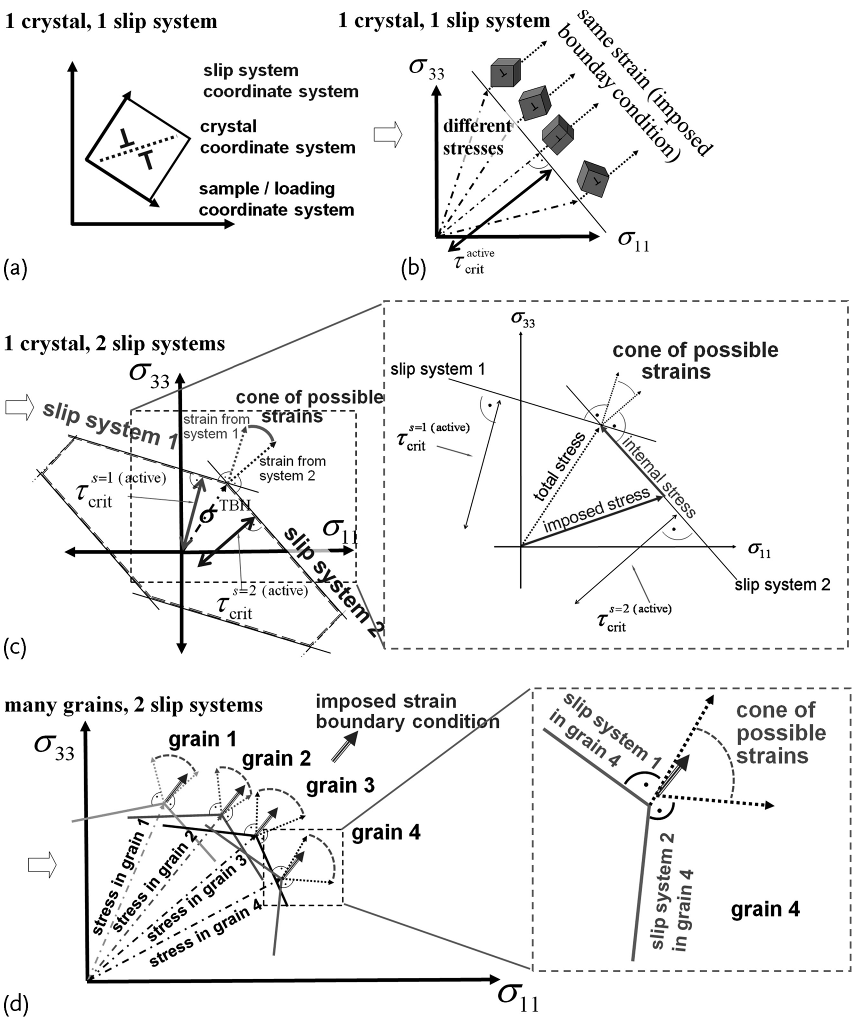


Figure 1.5 The increasing complexity of crystal-scale micromechanics with respect to the equilibrium of the forces and the compatibility of the displacements for different situations: (a, b) Single-slip situation in a single crystal presented in stress space. (c) Portion of a single-crystal yield surface with three slip systems. (d) Multislip situation in a polycrystal where all different crystals have to satisfy an assumed imposed strain in their respective yield corners. If the strain is homogeneous, this situation leads to different stresses in each crystal (Raabe *et al.*, 2002a, 2004a). τ_{crit}: critical shear stress; σ^{TBH}: Taylor–Bishop–Hill stress state (stress required to reach a yield corner).

suggested during the last few decades have gradually developed from empirical viscoplastic formulations (Asaro and Rice, 1977; Rice, 1971) into microstructure-based multiscale models of plasticity including a variety of size-dependent effects and interface mechanisms (Arsenlis and Parks, 1999, 2002; Arsenlis *et al.*, 2004; Cheong and Busso, 2004; Evers, Brekelmans, and Geers, 2004a,b; Evers *et al.*, 2002;

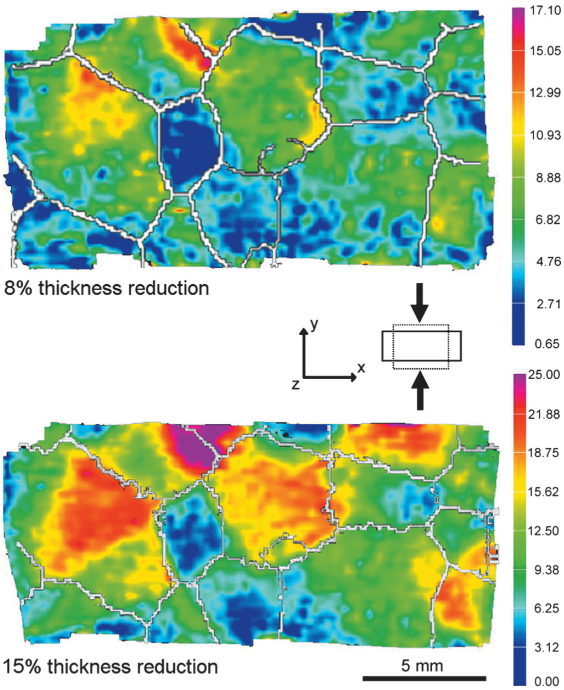


Figure 1.6 Experimental example of the heterogeneity of plastic deformation at the grain and subgrain scale using an aluminum oligocrystal with large columnar grains (Sachtleber, Zhao, and Raabe, 2002). The images show the distribution of the accumulated von Mises equivalent strain in a specimen after $\Delta y/y_0 = 8$ and 15% thickness reduction in plane strain (y_0 is the initial sample height). The experiment was conducted in a lubricated channel-die setup. White lines indicate high-angle grain boundaries derived from electron backscatter diffraction microtexture measurements. The equivalent strains (determined using digital image correlation) differ across some of the grain boundaries by a factor of 4–5, giving evidence of the enormous orientation-dependent heterogeneity of plasticity even in pure metals.

Ma and Roters, 2004; Ma, Roters, and Raabe, 2006a,b). In this context it should be emphasized that the finite element method itself is not the actual model but the variational solver for the underlying constitutive equations. Since its first introduction by Peirce *et al.* (1982), the CPFE method has matured into a whole family of constitutive and numerical formulations which have been applied to a broad variety of crystal mechanical problems. See Table 1.1 for examples and Roters *et al.* (2010) for a recent review.

In this book we give an overview of this exiting simulation method. In Part One we introduce the fundamentals of the approach by briefly reiterating the basics of the underlying metallurgical mechanisms, of continuum mechanics, and of the finite element method.

Subsequently, in Part Two, we discuss the details of classical and more advanced dislocation-based constitutive models which are currently used in this field. In this

Table 1.1 Some examples for different applications of the crystal plasticity finite element (CPFE) method.

Application of the CPFE method	References
Forming, deep drawing, process modeling, cup drawing, springback, earing, wire drawing, extrusion, anisotropy, design	Beaudoin *et al.* (1993), Beaudoin *et al.* (1994), Neale (1993), Kalidindi and Schoenfeld (2000), Nakamachi, Xie, and Harimoto (2001), Zhao *et al.* (2001), Xie and Nakamachi (2002), Raabe *et al.* (2002a) McGarry *et al.* (2004), Raabe and Roters (2004), Zhao *et al.* (2004a), Tugcu *et al.* (2004), Delannay *et al.* (2005), Li, Kalidindi, and Beyerlein (2005), Raabe, Wang, and Roters (2005), Tikhovskiy, Raabe, and Roters (2006), Delannay, Jacques, and Kalidindi (2006), Chen, Lee, and To (2007), Raabe (2007), Nakamachi, Tam, and Morimoto (2007), Ocenasek *et al.* (2007), Tikhovskiy, Raabe, and Roters (2007), Li, Donohue, and Kalidindi (2008c), Li *et al.* (2008b), Zhuang *et al.* (2008), Delannay *et al.* (2009), Zamiri, Bieler, and Pourboghrat (2009)
Surface roughening, ridging, roping, thin-film mechanics	Becker (1998), Raabe *et al.* (2003), Zhao, Radovitzky, and Cuitino (2004b), Yue (2005), Siska, Forest, and Gumbsch (2007), Zhao *et al.* (2008)
Damage, fatigue, cyclic loading, void growth, fretting	Bruzzi *et al.* (2001), Turkmen, Dawson, and Miller (2002), Goh, Neu, and McDowell (2003), Turkmen *et al.* (2003), Kysar, Gan, and Mendez-Arzuza (2005), Dick and Cailletaud (2006), Sinha and Ghosh (2006), Potirniche *et al.* (2006), Zhang and McDowell (2007), Cheong, Smillie, and Knowles (2007), Dunne, Walker, and Rugg (2007a), Liu *et al.* (2007), Bieler *et al.* (2009), Kumar *et al.* (2008), Mayeur, McDowell, and Neu (2008), Patil *et al.* (2008), Watanabe *et al.* (2008), McDowell (2008), Mayama, Sasaki, and Kuroda (2008), Borg, Niordson, and Kysar (2008)
Creep, high-temperature deformation, diffusion mechanisms	McHugh and Mohrmann (1997) Balasubramanian and Anand (2002), Hasija *et al.* (2003), Bower and Wininger (2004), Venkatramani, Ghosh, and Mills (2007), Agarwal *et al.* (2007), Venkataramani, Kirane, and Ghosh (2008), Xu *et al.* (2009)
Nanoindentation, pillar testing, microbending, microscale deformation, miniaturized mechanical testing	Wang *et al.* (2004), Zaafarani *et al.* (2006), You *et al.* (2006), Raabe, Ma, and Roters (2007a), Casals, Ocenasek, and Alcala (2007), Zaafarani *et al.* (2008), Alcala, Casals, and Ocenasek (2008), Weber *et al.* (2008), Xu *et al.* (2009), Demir *et al.* (2009)

Table 1.1 Some examples . . . (continued).

Application of the CPFE method	References
Grain boundary mechanics, Hall–Petch behavior, grain interaction, grain size effects, strain gradient effects, nonlocal formulations, interface mechanics, superplasticity	Becker and Panchanadeeswaran (1995) Mika and Dawson (1998), Acharya and Beaudoin (2000), Meissonnier, Busso, and O'Dowd (2001) Barbe *et al.* (2001), Raabe *et al.* (2001), Evers *et al.* (2002), Park *et al.* (2002), Clarke, Humphreys, and Bate (2003), Wei and Anand (2004), Fu, Benson, and Meyers (2004), Evers, Brekelmans, and Geers (2004a), Evers, Brekelmans, and Geers (2004b), Diard *et al.* (2005), Bate and Hutchinson (2005), Wei, Su, and Anand (2006), Murphy *et al.* (2006), Deka *et al.* (2006), Ma, Roters, and Raabe (2006a), Ma, Roters, and Raabe (2006b), Counts *et al.* (2008a), Gurtin, Anand, and Lele (2007), Venkatramani, Ghosh, and Mills (2007), Okumura *et al.* (2007), Gerken and Dawson (2008b), Gerken and Dawson (2008a), Kuroda and Tvergaard (2008a), Bitzek *et al.* (2008), Borg, Niordson, and Kysar (2008), Li *et al.* (2009)
In-grain texture formation, grain-scale mechanics, mesoscale, nonuniform deformation, texture evolution, texture stability, anisotropy	Peirce *et al.* (1982), Peirce, Asaro, and Needleman (1983), Asaro and Needleman (1985) Becker (1991), Becker *et al.* (1991), Bronkhorst, Kalidindi, and Anand (1992), Kalidindi, Bronkhorst, and Anand (1992), Beaudoin *et al.* (1995), Becker and Panchanadeeswaran (1995), Beaudoin, Mecking, and Kocks (1996), Beaudoin, Mecking, and Kocks (1996), Sarma and Dawson (1996b), Sarma and Dawson (1996a), Bertram, Böhlke, and Kraska (1997), Mika and Dawson (1998), Sarma, Radhakrishnan, and Zacharia (1998), Forest (1998), Mika and Dawson (1999), Miehe, Schröder, and Schotte (1999), Bhattacharyya *et al.* (2001), Raabe *et al.* (2001), Miller and Turner (2001), Kalidindi (2001), Balasubramanian and Anand (2002), Van Houtte, Delannay, and Kalidindi (2002), Delannay, Kalidindi, and Van Houtte (2002), Raabe, Zhao, and Mao (2002b), Raabe *et al.* (2002c) Sachtleber, Zhao, and Raabe (2002), Kim and Oh (2003), Clarke, Humphreys, and Bate (2003), Choi (2003), Zaefferer *et al.* (2003), Erieau and Rey (2004), Roters *et al.* (2004), Bate and An (2004), Raabe, Zhao, and Roters (2004b), Li, Van Houtte, and Kalidindi (2004), Sarma and Radhakrishnan (2004), Anand (2004), Roters, Jeon-Haurand, and Raabe (2005), Van Houtte *et al.* (2005), Li, Kalidindi, and Beyerlein (2005), Van Houtte *et al.* (2006), Delannay, Jacques, and Kalidindi (2006), Tang *et al.* (2006), Tikhovskiy, Raabe, and Roters (2006), Kim and Oh (2006), Murphy *et al.* (2006), daFonseca *et al.* (2006), You *et al.* (2006), Musienko *et al.* (2007), Han and Dawson (2007), Lee, Wang, and Anderson (2007), Tikhovskiy, Raabe, and Roters (2007), Zhao *et al.* (2008), Mayeur, McDowell, and Neu (2008), Delannay *et al.* (2009) Zhang *et al.* (2009)

Table 1.1 Some examples . . . (continued).

Application of the CPFE method	**References**
Dislocation-based constitutive modeling	Arsenlis and Parks (1999), Arsenlis and Parks (2002), Arsenlis and Tang (2003), Arsenlis *et al.* (2004), Evers *et al.* (2002), Evers, Brekelmans, and Geers (2004b), Cheong and Busso (2004), Ma and Roters (2004), Evers, Brekelmans, and Geers (2004a), Ma, Roters, and Raabe (2006a), Ma, Roters, and Raabe (2006b), McDowell (2008), Li *et al.* (2009)
Deformation twinning	Kalidindi (1998), Staroselsky and Anand (1998), Marketz *et al.* (2002), Staroselskya and Anand (2003), Marketz, Fischer, and Clemens (2003), Salem, Kalidindi, and Semiatin (2005)
Martensite mechanics, phase transformation, shape memory	Marketz and Fischer (1994), Marketz and Fischer (1995), Tomita and Iwamoto (1995), Diani, Sabar, and Berveiller (1995), Diani and Parks (1998), Cherkaoui, Berveiller, and Sabar (1998), Cherkaoui, Berveiller, and Lemoine (2000), Thamburaja and Anand (2001), Tomita and Iwamoto (2001), Govindjee and Miehe (2001), Anand and Gurtin (2003), Turteltaub and Suiker (2005), Thamburaja (2005), Lan *et al.* (2005), Turteltaub and Suiker (2006b), Tjahjanto, Turteltaub, and Suiker (2008), Geers and Kouznetsova (2007),
Multiphase mechanics	Hartig and Mecking (2005), Tjahjanto, Roters, and Eisenlohr (2007), Mayeur, McDowell, and Neu (2008), Inal, Simha, and Mishra (2008), Vogler and Clayton (2008)
Crystal plasticity and recrystallization	Bate (1999), Raabe and Becker (2000), Raabe (2000), Radhakrishnan *et al.* (2000), Raabe (2002), Takaki *et al.* (2007), Raabe (2007), Semiatin *et al.* (2007), Zambaldi *et al.* (2007), Loge *et al.* (2008)
Numerical aspects, finite element shape effects, mesh dependence, accuracy, robust integration methods, texture discretization	Miehe (1996), Bachu and Kalidindi (1998), Harewood and McHugh (2006), Amirkhizi and Nemat-Nasser (2007), Harewood and McHugh (2007), Kuchnicki, Cuitino, and Radovitzky (2006), Melchior and Delannay (2006), Zhao *et al.* (2007), Li, Yang, Sun (2008a), Eisenlohr and Roters (2008), Ritz and Dawson (2009), Barton *et al.* (2004), Gerken and Dawson (2008b)

context we explain the representation of dislocation slip, displacive transformations such as martensite formation and mechanical twinning, and the failure mechanism within such a variational framework. Also, we address homogenization and numerical aspects associated with the finite element solution of crystal plasticity problems.

Finally, Part Three presents a number of microscopic, mesoscopic, and macroscopic applications from the field of CPFE modeling.