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Crystal Plasticity Finite Element Method (CPFEM): state-of-the-art

Abstract: A brief discussion is given for crystal plasticity finite element method, reasons of its importance and its microscopic and macroscopic applications. Also, discussions were made for its primary engineering objectives and its further related applications. Chronological brief of evolution of its two legs: finite element method and crystal plasticity was also captured. Chronological brief of necessities and developments of new models was also tracked.

Keywords: Crystal plasticity, Twinning, Indentation, Multiphase steel, Anisotropy.

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Introduction

Why crystal plasticity finite-element method

Loading direction controls elastic plastic deformation of crystalline materials, i.e. mechanical anisotropy behavior dominates crystal behavior subjected to various mechanical loadings. The reasons for that are not only that elastic tensor is anisotropic, but also because the activation of crystallographic deformation mechanisms (dislocations, twins, martensitic transformations) is orientation dependent. Consequently, the associated mechanical phenomena such as shape change, crystallographic texture, strength, strain hardening, deformation-induced surface roughening and damage are all orientation dependent. This leads to an important result: the mechanical parameters of crystalline materials are tensor quantities (Roters, et al., 2010)).

This leads to two important facts. The first fact is that the uniaxial stress-strain curve, which is believed to have been practiced since Greek Procrustes or even before him thousands of years ago (Answers, 2023), is no longer enough to describe plastic deformation phenomena (Figure 1). The second fact is that plastic deformation influences crystallographic texture and its evolution during forming. Hence, integral anisotropy of polycrystals can be described by texture i.e. individual tensorial behavior of each grain and the orientation-dependent boundary conditions among the crystals can be used to describe integral plasticity.

Incorporating present knowledge of deformation physics (Curtin & Miller, 2003), (Arsenlis, Parks, Becker, & Bulatov, 2004) and (Vitek, Mrovec, & Bassani, 2004) into the computational tools of continuum mechanics (Zienkiewicz, 1967), (Zienkiewicz & Taylor, 2005) aiming to develop physically based advanced design methods that can be used in engineering application.

Early approaches in the West to describe anisotropic plasticity under simple boundary conditions have considered these aspects, such as, for instance, (Sachs, 1928), (Taylor, 1938), (Bishop & Hill, 1951), (Bishop & Hill, 1951) or (Kro¨ner, 1961) formulations.

Early approaches, in Russia, to the development of physics and physical chemistry plastic deformation was introduced by domestic scientists V.D. Kuznetsov, N.S. Kurnakov, N.N. Davidenko, A.A. Bochvar, S.I. Gubkin.

There were interactions between the two sides. Many of works of the following western scientists have been translated into Russian language: J. Alexander, J. Bishop, P. Bridgman, V. Bakofen, O. Goffman, V. Johnson, G. Sachs, Sh. Kobayashi, H. Kudo, A. Nadai, H. Pugh, E. Thomsen, R. Hill, K. Young, and other. Also, there were attention in the west about Russian efforts in this field. Proves that, the inclusion of Russia (that time called Soviet Union) and Russian language in related scientific associations since its early foundation, such as IDDRG (International Deep Drawing Research Group) since its early foundation in 1960 (BrDDRG, 2022).

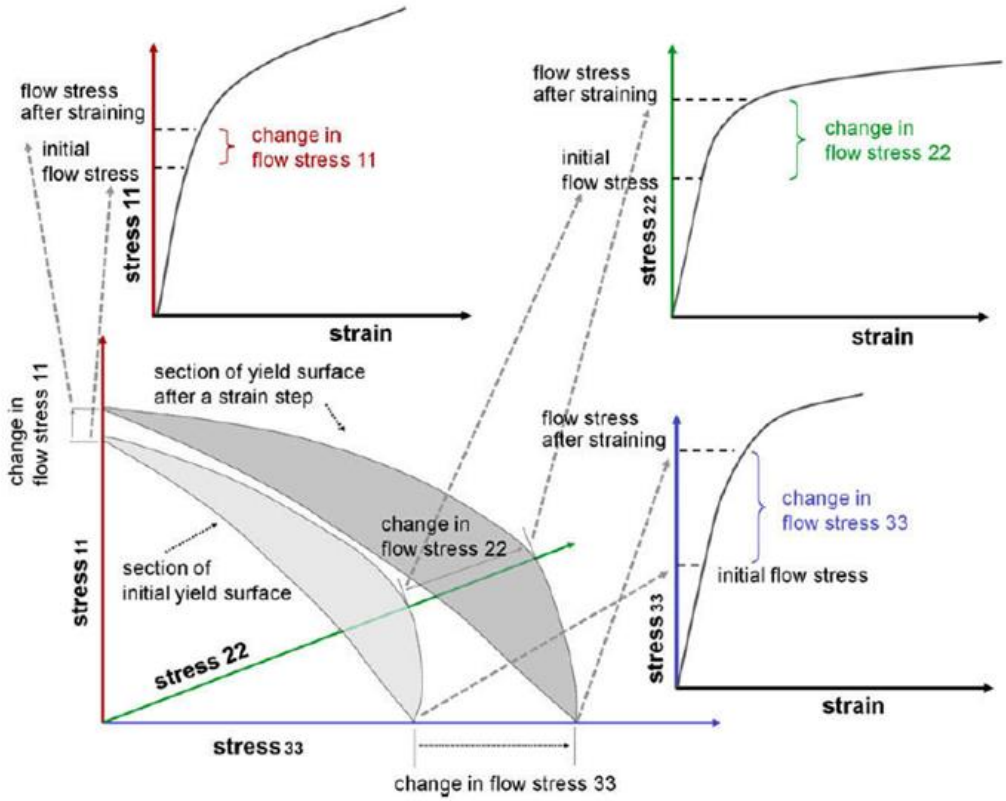

Figure 1. Flow stress and strain hardening of anisotropic materials are, merely, tensor quantities

In the development of the theory of plasticity, four can be distinguished:

1. **The first period:** Characteristic period was approximately from 1915 to 1945. The simplest ones have been solved problems based on general equations of plasticity theory for determining the strength of the most common metal forming operations (S.I. Gubkin, G. Sachs, E. Siebel, N.S. Petrov, L. Prandtl, E.P. Unksov, A.I. Tselikov).
2. **Second period:** (approximately from 1945 to 1960). Development of general approximate methods for solving problems related to determining deformation forces, tool loads and final forming. Engineering methods for analyzing mechanical engineering processes has been developed (S.I. Gubkin, G. Sachs, E. Siebel, I.M. Pavlov, E.A. Popov, V.S. Smirnov, M.V. Storozhev, E.P. Unksov), sliding line method (G. Genki, H. Geiringer, W. Prager, I.P. Renne, V.V. Sokolovsky, A.D. Tomlenov, R. Hill, L.A. Shofman), energy method (O.A. Ganago, V. Johnson, W.L. Kolmogorov, A.A. Pozdeev, I.Ya. Tarnovsky, E. Thomsen), method of resistance of metals to plastic deformation (G.A. Smirnov-Alyaev), visioplastic (Yu.N. Alekseev, E. Thomsen).
3. **Third period**: (approximately from 1960 to 1975). Development of methods used theoretical analysis of mechanical engineering processes by numerical methods and computers. The prerequisites have been created for the construction and analysis of models of metal forming processes that more fully take into account real conditions of deformation, and solving new problems in extreme shape change. Secondly, through the efforts of leading Scientists in Russia have created scientific schools, in particular:
    - Moscow (A.A. Ilyushin, N.N. Malinin, E.A. Popov, M.V. Storozhev, A.D. Tomlenov, E.P. Unksov, L.A. Shofman, V.T. Meshcherin, I.A. Noritsyn);

- Leningrad (V.S. Smirnov, G.A. Smirnov-Alyaev), Ural (O.A. Ganago, V.L. Kolmogorov, A.A. Pozdeev, A.A. Bogatov, I.Ya. Tarnovsky);
- Minsk (E.M. Makushok, V.P. Severdenko, V.M. Segal), Tula (I.P. Renne, L.A. Tolokonnikov, S.P. Yakovlev);
- Kharkov (Yu.N. Alekseev, E.F. Sharapov, V.A. Evstratov);
- Rostov (A.Z. Zhuravlev);
- Oryol (V.A. Golenkov).

4. **The fourth period:** (since approximately 1975). In this period, the works that deserve attention are those of G.D. Delya, E.I. Isachenkova, A.N. Levanova, V.L. Kol-mogorova, P.I. Polukhina, G.Ya. Guna, A.M. Galkina, G.A. Smirnova-Alyaeva, V.I. Uralsky, N.A. Chichenova, A.B. Kudrina. In them, the theoretical approach is based on experimental data, their statistical analysis, the use of new ideas about contact friction and material destruction, the role temperature, speed and mechanical deformation patterns.

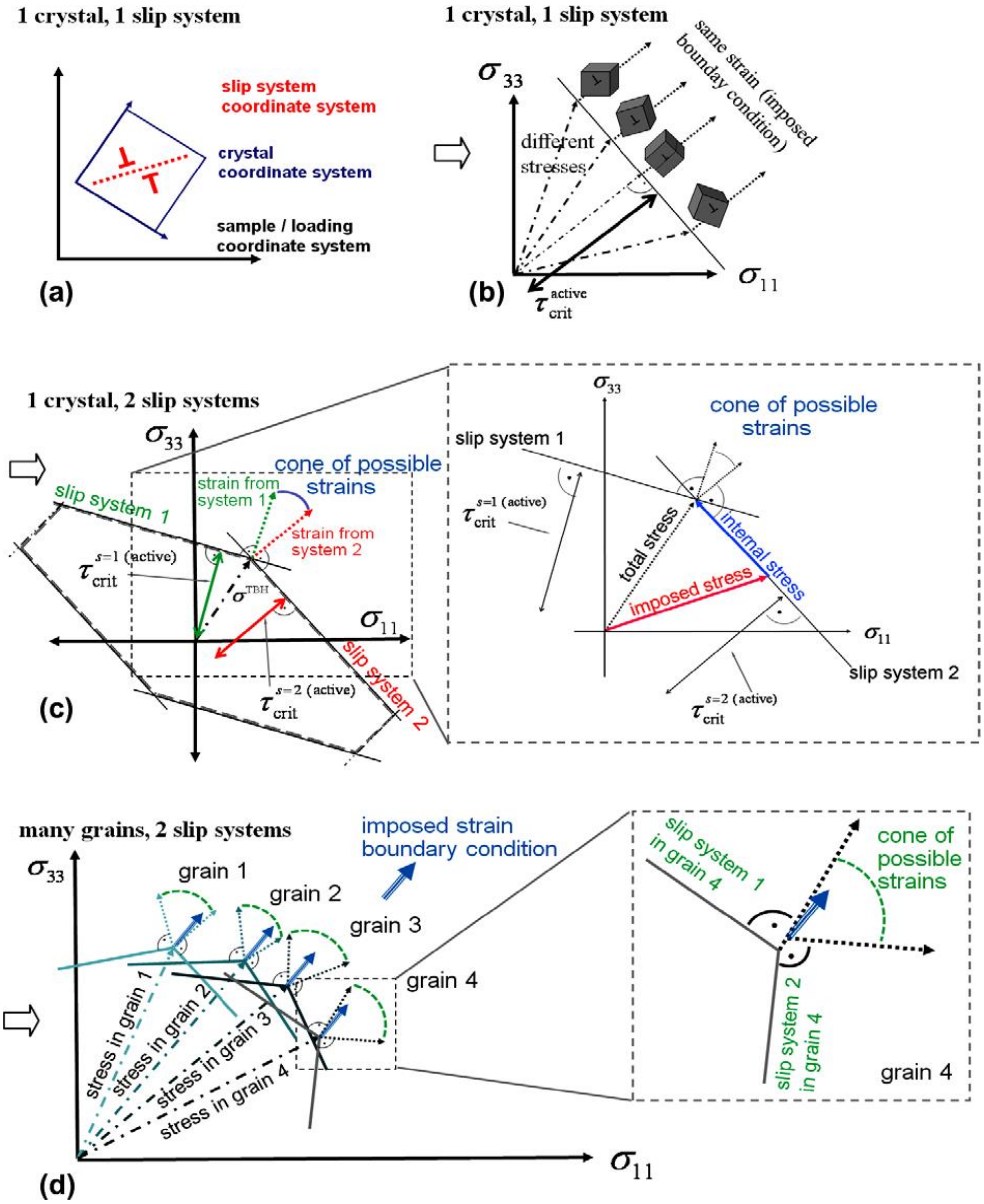

Figure 2. Schematically presented growing complexity of grain-scale mechanics with respect to the equilibrium of the forces and the compatibility of the displacements for different situations (a and b). Single slip problem in a single crystal presented in stress space (c). Part of a single-crystal yield surface with two slip systems (d). Multi-slip situation in a polycrystal where all different crystals must satisfy an assumed imposed strain in their respective yield corners. According to (Raabe, et al., 2002), (Raabe, Roters, Barlat, & Chen, 2004), different stresses in each crystal, τ_{critic}: critical shear stress, σ^{TBH}: Taylor–Bishop–Hill stress state (stress required to reach a yield corner), results from the situation of strain homogeneity.

However, the approaches of both Western and Russian scientists, in the first and second periods and to some extent third period, were neither designed for responding to complex internal or external boundary conditions nor considering explicitly the mechanical interactions among the crystals in a polycrystal (Figure 2). 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, in the fourth period, enormous momentum was given to variational methods such as finite element approximations. 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 ability to solve crystal mechanical problems under complicated internal and/or external boundary conditions is one of CPFE main advantages. Since, it enables to tackle those boundary conditions that are imposed by inter- and intra-grain micromechanical interactions (

Figure **3**) (Sachtleber, Zhao, & Raabe, 2002), this aspect is not a mere computational advantage but is an inherent part of the physics of crystal mechanics. 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, Sachtleber, Weiland, Scheele, & Zhao, 2003).

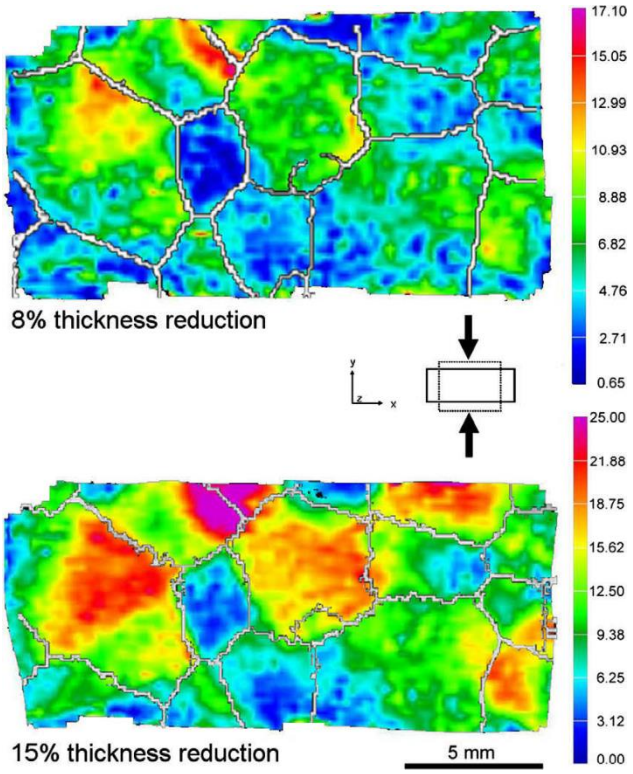

Figure 3. Experimental example of the heterogeneity of plastic deformation at the grain and subgrain scale using an aluminum polycrystal with large columnar grains (Sachtleber, Zhao, & Raabe, 2002). The equivalent strains differ across some of the grain boundaries by a factor of 4–5, giving evidence of the enormous orientation-dependent heterogeneity of plasticity even in pure metals. The images show the distribution of the accumulated von Mises equivalent strain in a specimen after 8% and 15% plane strain sample thickness reduction (the deformation is given in % of $\Delta d/d$, where d is the sample extension along compression direction). The experiment was conducted in a lubricated channel–die set-up. The strains were determined using digital image correlation. The high-angle grain boundaries indicated by white lines were taken from electron backscatter diffraction microtexture measurements.

CPFE methods have several advantages. Firstly, they, efficiently, deal with complicated boundary conditions. Secondly, they also offer, at the elementary shear system level, great flexibility with respect to including various constitutive formulations for plastic flow and hardening. The constitutive flow laws that were suggested during the last decades have gradually developed from empirical viscoplastic formulations (Rice, 1971) (Asaro & Rice, 1977) into physics-based multiscale internal-variable models of plasticity, including a variety of size-dependent effects and interface mechanisms (Arsenlis, Parks, Becker, & Bulatov, 2004), (Arsenlis

& Parks, 1999), (Arsenlis & Parks, 1999), (Evers, Brekelmans, & Geers, 2004). The CPFE method has matured into a whole family of constitutive and numerical formulations that has been applied to a broad variety of crystal mechanical problems (**Table 1**). This is the accumulation of works since it was firstly introduced by (Peirce, Asaro, & Needleman, 1982).

1.2. Aspects of crystal plasticity finite-element method

1. **Handling various dyadic kinematics mechanisms:** CPFE approach can handle various dyadic kinematics mechanisms such as dislocation, martensite formation (Thamburaja & Iwamoto, 2001), (Lan, Xiao, Li, & Li, 2005), shear band formation (e.g. in glassy matter) (Anand & Sun, 2005), mechanical twinning (Kalidindi S. R., 1998), (Staroselsky & Anand, 1998), (Marketz W. T., et al., 2002), (Salem, Kalidindi, & Semiatin) and superplastic grain boundary shear (Wei & Anand, 2004), (Wei, Su, & Anand, 2006). This means that a type of deformation mechanism (e.g. dislocation slip) may occur at some material point while in another point several mechanisms (e.g. dislocations and twins) may appear together;

Table 1. Examples for different applications of the CPFE method

Application of the CPFE method	Reference
Surface roughening, roping, ridging, thin film mechanics	(Becker, 1998), (Raabe, Sachtleber, Weiland, Scheele, & Zhao, 2003), (Zhao, Radovitzky, & Cuitino, 2004), (Yue, 2005), (Siska, Forest, & Gumbsch, 2007), (Zhao, Ramesh, Raabe, Cuitino, & Radovitzky, 2008)
Grain boundary mechanics, grain interaction, grain size effects, strain gradient effects, non-local formulations, interface mechanics, superplasticity, Hall–Petch behaviour, strain gradient effects	(Wei & Anand, 2004), (Fu, Benson, & Meyers, 2004), (Evers, Brekelmans, & Geers, 2004), (Evers, Brekelmans, & Geers, 2004), (Diard, Leclercq, Rousselier, & Cailletaud, 2005), (Bate & Hutchinson, 2005), (Wei, Su, & Anand, 2006), (Murphy, Cuddy, Harewood, Connolley, & McHugh, 2006), (Deka, Joseph, Ghosh, & Mills, 2006), (Ma, Roters, & Raabe, 2006) (Ma, Roters, & Raabe, 2006), (Gurtin, Anand, & Lele, 2007), (Venkatramani, Ghosh, & Mills, 2007), (Okumura, Higashi, Sumida, & Ohno, 2007), (Gerken & Dawson, 2007), (Counts, Braginsky, Battaile, & Holm, 2008), (Gerken & Dawson, 2008), (Kuroda & Tvergaard, 2008), (Bitzek, Derlet, Anderson, & Van Swygenhoven, 2008), (Borg, Niordson, Kysar, & Kysar, 2008), (Li, et al., 2009)
Creep, high temperature deformation, diffusion mechanisms	(McHugh & Mohrmann, 1997), (Balasubramanian & Anand, 2002), (Hasija, Ghosh, Mills, & Joseph, 2003), (Bower & Wininger, 2004), (Venkatramani, Ghosh, & Mills, 2007), (Agarwal, Briant, Krajewski, Bower, & Taleff, 2007), (Venkataramani, Kirane, & Ghosh, 2008), (Xu, Yonezu, Yue, & Chen, 2009)
Dislocation-based constitutive modelling	(Marketz & Fischer, 1994), (Arsenlis & Parks, 1999), (Arsenlis & Parks, 2002), (Evers, Parks, Brekelmans, & Geers, 2002), (Arsenlis & Tang, 2003), (Arsenlis, Parks, Becker, & Bulatov, 2004), (Evers, Brekelmans, & Geers, 2004), (Cheong & Busso, 2004), (Evers, Brekelmans, & Geers, 2004), (Ma & Roters, 2004), (Ma, Roters, & Raabe, 2006), (Ma, Roters, & Raabe, 2006), (McDowell, 2008)
Martensite mechanics, phase transformation, shape memory	(Marketz & Fischer, 1994), (Marketz & Fischer, 1995), (Tomita & Iwamoto, 1995), (Diani, Sabar, & Berveiller, 1995), (Diani & Parks, 1998), (Cherkaoui, Berveiller, & Sabar, 1998), (Cherkaoui, Berveiller, & Lemoine, 2000), (Thamburaja & Anand, 2001), (Tomita & Iwamoto, 2001), (Govindjee & Miehe, 2001) (Anand & Gurtin, 2003), (Turteltaub & Suiker, 2005), (Thamburaja, 2005), (Lan, Xiao, Li, & Li, 2005), (Turteltaub & Suiker, 2006), (Geers & Kouznetsova, 2007), (Tjahjanto, Turteltaub, & Suiker, 2008)
In-grain texture, grain-scale mechanics, non-uniform	(Sarma, Radhakrishnan, & Zacharia, 1998), (Forest, 1998), (Bhattacharyya, El-Danaf, Kalidindi, & Doherty, 2001), (Raabe, Sachtleber,

deformation, grain-scale mechanics, mesoscale	Zhao, Roters, & Zaefferer, 2001), (Miller & Turner, 2001), (Raabe, Zhao, Park, & Roters, 2002), (Sachtleber, Zhao, & Raabe, 2002), (Kim & Oh, 2003), (Clarke, Humphreys, & Bate, 2003), (Choi, 2003), (Zaefferer, Kuo, Zhao, Winning, & Raabe, 2003), (Erieau & Rey, 2004), (Sarma & Radhakrishnan, 2004), (Roters, Wang, Kuo, & Raabe, 2004), (Kim, Kim, & Oh, 2006), (Murphy, Cuddy, Harewood, Connolley, & McHugh, 2006)], (daFonseca, Oliver, Bate, & Withers, 2006), (You, Connolley, McHugh, & Motz, 2006), (Musienko, et al., 2007), (Han & Dawson, 2007), (Zhao, Ramesh, Raabe, Cuitino, & Radovitzky, 2008), (Zhang, Bower, Mishra, & Boyle, 2009)
Texture evolution, texture stability, anisotropy, in-grain texture formation	(Mika & Dawson, 1999), (Miehe, Schro¨der, & Schotte, 1999), (Kalidindi S. R., 2001), (Balasubramanian & Anand, 2002), (Van Houtte, Delannay, & Kalidindi, 2002) (Delannay, Kalidindi, & Van Houtte, 2002), (Raabe, Zhao, & Mao, 2002), (Bate & An, 2004), (Raabe, Zhao, & Roters, 2004), (Li, Van Houtte, & Kalidindi, 2004), (Sarma & Radhakrishnan, 2004), (Anand, 2004), (Roters, Jeon-Haurand, & Raabe, 2005), (Van Houtte, Van Bael, Seefeldt, & Delannay, 2005), (Li, Kalidindi, & Beyerlein, 2005), (Van Houtte, Kanjarla, Van Bael, Seefeldt, & Delannay, 2006), (Delannay, Jacques, & Kalidindi, 2006), (Tang, Zhang, Chen, & Deng, 2006), (Tikhovskiy, Raabe, & Roters, 2006), (Lee, Wang, & Anderson, 2007), (Tikhovskiy, Raabe, & Roters, 2007), (Mayeur, McDowell, & Neu, 2008), (Delannay, Melchior, Signorelli, Remacle, & Kuwabara, 2009)
Forming, deep drawing, cup drawing, process modelling, spring-back, earing, anisotropy, wire drawing, extrusion, design, fretting	(Zhao, Mao, Roters, & Raabe, 2004), (Tugcu, Neale, Wu, & Inal, 2004), (Delannay, Beringhier, Chastel, & Loge, 2005), (Raabe, Wang, & Roters, 2005), (Dick & Cailletaud, 2006), (Delannay, Jacques, & Kalidindi, 2006), (Tikhovskiy, Raabe, & Roters, 2007), (Chen, Lee, & To, 2007), (Raabe, 2007), (Nakamachi, Tam, & Morimoto, 2007), (Ocenasek, Rodriguez Ripoll, Weygand, & Riedel, 2007), (Tikhovskiy, Raabe, & Roters, 2007), (Li, Donohue, & Kalidindi, 2008), (Mayeur, McDowell, & Neu, 2008), (Li, Donohue, & Kalidindi, 2008), (Li, et al., 2008), (Zhuang, Wang, Cao, Lin, & Hart, 2008), (Delannay, Melchior, Signorelli, Remacle, & Kuwabara, 2009), (Zamiri, Bieler, & Pourboghrat, 2009)
Crystal plasticity and recrystallization	(Bate P. , 1999), (Raabe & Becker, 2000), (Raabe, 2000), (Radhakrishnan, Sarma, Weiland, & Baggethun, 2002), (Raabe, 2002), (Takaki, Yamanaka, Higa, & Tomita, 2007), (Raabe, 2007), (Semiatin, Weaver, Goetz, Thomas J., & Turner, 2007), (Zambaldi, Roters, Raabe, & Glatzel, 2007), (Loge, et al., 2008)
Deformation twinning	(Kalidindi S. R., 1998), (Staroselsky & Anand, 1998), (Marketz W. T., et al., 2002), (Staroselskya & Anand, 2003), (Marketz, Fischer, & Clemens, 2003), (Salem, Kalidindi, & Semiatin, Strain hardening due to, 2005)
Nanoindentation, pillar testing, micro-scale deformation, micro-bending, testing	(Wang, Raabe, Klu¨ber, & Roters, 2004), (Zaafarani, Raabe, Singh, Roters, & Zaefferer, 2006), (You, Connolley, McHugh, & Motz, 2006), (Raabe, Ma, & Roters, 2007), (Casals, Ocenasek, & Alcala, 2007), (Zaafarani, Raabe, Roters, & Zaefferer, 2008), (Alcala, Casals, & Ocenasek, 2008), (Weber, Schestakow, Roters, & Raabe, 2008), (Xu, Yonezu, Yue, & Chen, 2009), (Demir, Raabe, Zaafarani, & Zaefferer, 2009)
Numerical aspects, FE shape effects, mesh dependence, texture discretization, accuracy, robust integration methods	(Miehe, 1996), (Bachu & Kalidindi, 1998), (Harewood & McHugh, 2006), (Kuchnicki, Cuitino, & Radovitzky, 2006), (Amirkhizi & Nemat-Nasser, 2007), (Harewood & McHugh, 2007), (Melchior & Delannay, 2006), (Zhao, Kuchnicki, Radovitzky, & Cuitin˜o, 2007), (Li, Yang, & Sun, 2008), (Ritz & Dawson, 2009), (Barton, et al., 2001), (Gerken & Dawson, 2007)

Damage, cyclic loading, void growth, fatigue	(Bruzzi, McHugh, O'Rourke, & Linder, 2001), (Turkmen, Dawson, & Miller, 2002), (Turkmen, Loge, Dawson, & Miller, 2003), (Kysar, Gan , & Mendez-Arzuza, 2005), (Sinha & Ghosh, 2006), (Potirniche, Hearndon, Horstemeyer, & Ling, 2006), (Zhang, Zhang, & McDowell, 2007), (Cheong, Smillie, & Knowles, 2007), (Dunne, Walker, & Rugg, 2007), (Liu, Zhang, Tang, & Du, 2007), (Kumar, et al., 2008), (Patil, Narasimhan , Biswas, & Mishra, 2008), (Watanabe, Terada, deSouza, & Peric, 2008), (McDowell, 2008), (Mayama, Sasaki, & Kuroda M., 2008), (Borg, Niordson, Kysar, & Kysar, 2008), (Bieler , et al., 2009)
Multiphase mechanics	(Hartig & Mecking, 2005), (Tjahjanto, Roters, & Eisenlohr, 2007), (Mayeur, McDowell, & Neu, 2008), (Inal, Simha, & Mishra, 2008) (Vogler & Clayton, 2008)

2. **Sub-models necessity:** Complexity in the latter case arises from the necessity of sub-models to describe the evolving fractions (e.g. of the twinned volume) and the interaction between various mechanisms at the same field point (Figure 4);
3. **Complexity increase:** Martensite or twins may, after their formation, undergo:
   - Further plastic deformation;
   - Create accommodation strains related to volume changes;
4. **Interactions implementation:** The user of CPFE can not only implement these shear mechanisms, but also their interactions;
5. **Local homogenization rules:** The resulting complexity requires the formulation of local homogenization rules (Raabe, et al., 2002), (Raabe & Roters, 2004);
6. **Close connection:** CPFE method includes close connection between shape change, rotation and geometrically necessary dislocations (GNDs) (Nye, 1953), (Kroner, 1958), (Ashby, 1970), (Kroner, 1981);
7. **Constitutive laws implementation:** This allows implementing constitutive laws that treat mechanical size effects in conjunction with local orientation gradients (Ma, Roters, & Raabe, 2006);
8. **Size-dependent plasticity modeling:** This point is relevant to size-dependent plasticity modeling, as the polarized portions of dislocation arrays (which are often conceptually treated as GNDs), such as anticipated in many size effects models, must necessarily coincide with orientation gradients (Nye, 1953);
9. **High Resolution Measurements:** Nowadays, it is possible to measure, precisely and in 2D and 3D high resolution measurements, such lattice rotations. This leads to the possibility of testing corresponding models (Larson, et al., 2002), (Kuo, Zaefferer, Zhao, Winning, & Raabe, 2003), (Zaefferer, Kuo, Zhao, Winning, & Raabe, 2003), (Roters, Wang, Kuo, & Raabe, 2004), (Zaafarani, Raabe, Singh, Roters, & Zaefferer, 2006), (Zaefferer, Wright, & Raabe, 2008), (Demir, Raabe, Zaafarani, & Zaefferer, 2009).
10. **Homogenization schemes:** Appropriate homogenization schemes are required within a CPFE model. That is because a larger number of crystals and/or phases must be considered in each representative volume element mapped at a FE integration point.
11. **Numerical aspects:** Numerical aspects also deserve attention. CPFE formulations can be either fully integrated into FE codes or implemented as user-defined subroutines into commercially available solvers. The latter case is important because engineering applications are often tackled using commercial platforms. The use of standard solvers also helps to make CPFE methods accessible to a broader community.
12. **Mesh and the integration procedures**: They also play a significant role in CPFE simulations.

The possibility of using CPFE modelling in both microscopic and macroscopic scales is another advantage (Raabe, et al., 2002).

1.2.1 Microscopic applications of CPFE

1. Inter- and intra-grain mechanics, damage initiation, mechanics at interfaces, simulation of micromechanical experiments (e.g. indentation, pillar compression, beam bending);
2. Prediction of local lattice curvatures and mechanical size effects (Table 1);

3. CPFE simulations for experimental boundary conditions in small-scale material testing. In such testing, it is difficult to control and/or monitor experimental boundary conditions and sometimes it is difficult to interpret experimental results without corresponding CPFE simulations. It allows the experimentalist to simulate the effects of details in the contact and boundary conditions;
4. Engineering design of grain scaled parts, e.g. microelectromechanical systems (MEMS), bonding wires and pillars, stents, and practically all materials in electronic components. Design of such parts increasingly requires consideration of grain-scale crystalline anisotropy.

1.2.1 Macroscopic applications of CPFE

Primary engineering objectives of CPFE applications in macroscopic forming simulations are the prediction of:

1. The precise material shape after forming;
2. Thickness distribution;
3. Material failure;
4. Optimization of material flow (Kraska, Doig, Tikhomirov , Raabe, & Roters, 2009);
5. Elastic spring-back;
6. Forming limits (Nakamachi, Xie, & Harimoto, 2001), (Xie & Nakamachi, 2002);
7. Texture evolution (Zhao, Mao, Roters, & Raabe, 2001), (Zhao, Mao, Roters, & Raabe, 2004), (Raabe, Wang, & Roters, 2005);
8. Mechanical properties of the formed part.

Further related applications occur in:

1. Virtual mechanical laboratory (Kraska, Doig, Tikhomirov , Raabe, & Roters, 2009);
2. Press layout;
3. Tool design;
4. Surface properties (Table 1);
   - Macroscopic (e.g. wrinkling);
   - Microstructural (e.g. roping, ridging, orange peel) mechanisms that influence the surface topography (Raabe, Sachtleber, Weiland, Scheele, & Zhao, 2003), (Becker, 1998), (Zhao, Radovitzky, & Cuitino, 2004).

2. Chronological brief

2.1. Finite Element (FE):

1. The first FE simulation was performed by Courant in 1943 [218].
2. The breakthrough of the method came with the publication of "The Finite Element Method in Structural and Continuum Mechanics" by (Zienkiewicz, 1967).
3. The three succeeding volumes (Zienkiewicz & Taylor, 2005), (Zienkiewicz, Taylor, & Zhu, 2005), (Zienkiewicz, Taylor, & Nithiarasu, 2005) are considered the most important monographs in the field to date.

2.2 Crystal Plasticity (CP)

1. Despite that, it has been known since 1934 (Taylor, 1934), (Orowan, 1934), (Polanyi, 1934) that crystalline materials deform plastically by the slip of dislocations on discrete slip systems, for a long-time continuum mechanical FE simulation used isotropic material models;
2. The first CPFE simulations were performed by (Peirce, Asaro, & Needleman, 1982). Due to computational restrictions they used a simplified set-up of two symmetric slip systems in order to study the tensile behavior of a single crystal;
3. These simulations were later extended to a polycrystalline arrangement by (Harren, De`ve, & Asaro, 1988), (Harren & Asaro, 1989) using a 2D setup with two or three slip systems;
4. In 1991 Becker was the first to perform simulations based on the 12 slip systems of a face-centered cubic (fcc) crystal. Using a 3D model for the crystallographic degrees of freedom, he simulated channel–die deformation of a columnar polycrystal aggregate (Becker, 1991) and of a single crystal (Becker, Butler, Hu, & Lalli, 1991);
5. In the field of direct or one-to-one crystal plasticity models numerous grain- and subgrain scale problems have been tackled using meshes with sub grain resolutions and, in part, complex 2D and 3D grain arrangements (Sachtleber, Zhao, & Raabe, 2002), (Siska, Forest, & Gumbsch, 2007), (Mika & Dawson, 1998), (Sarma & Dawson , 1996), (Sarma, Radhakrishnan, & Zacharia,

1998), (Beaudoin, Mecking, & Kocks, 1996), (Bachu & Kalidindi, 1998), (Zhao, Kuchnicki, Radovitzky, & Cuitin˜o, 2007);

6. On the macroscopic side, homogenization schemes were developed for the application of the CPFE method to large-scale forming operations. In this case the main problem was the correct representation of the (statistical) crystallographic texture of the material in the CPFE mesh. This can be achieved in different ways using, for example, texture components (Zhao, Mao, Roters, & Raabe, 2001), (Raabe & Roters, 2004) or direct sampling of single orientations from the orientation distribution function (ODF) (Melchior & Delannay, 2006), (To´th & Van Houtte, 1992), (Eisenlohr & Roters, 2008).

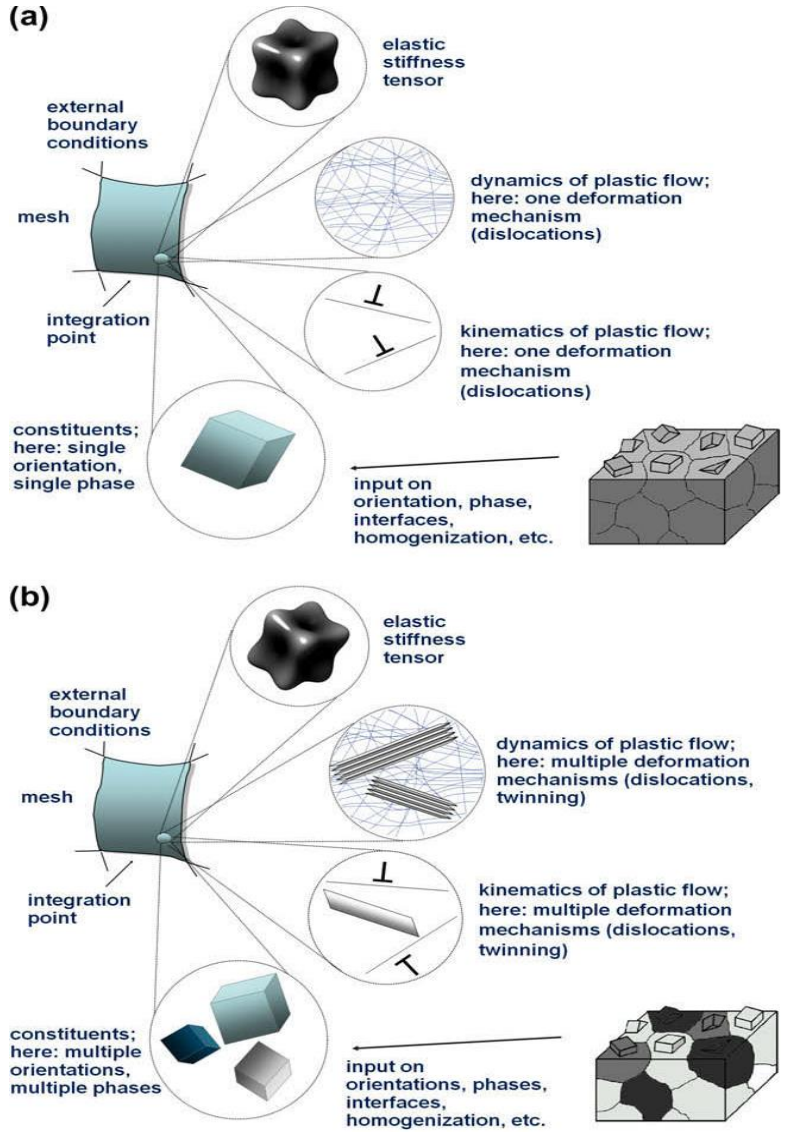

Figure 4. Schematic presentation of the conceptual ingredients in CPFE simulations. (a) Example of a case with one type of deformation mechanism (lattice dislocations) and one phase. (b) Example of a case with various deformation mechanisms, phases, orientations and homogenization schemes at the same integration point.

2.3 New Models

Phenomenological strain gradient theories were developed by (Fleck, Muller, Ashby, & Hutchinson, 1994), (Fleck & Hutchinson, 1997.), and (Nix & Gao, 1998). Using these theories, size effects can be introduced into CPFE frameworks. Also, because strain gradients can be associated with GNDs, new internal-variable constitutive formulations were developed that incorporate dislocation densities as physically based state variables (Arsenlis & Parks, 2002), (Arsenlis & Parks, 1999), (Arsenlis & Parks, 2002), (Ma, Roters, & Raabe, 2006), (Ma, Roters, & Raabe, 2006), (Gao & Huang, 2003) instead of strain measures, which were often used in phenomenological formulations.

Additional metallurgical mechanisms can be incorporated due to those most recent class of constitutive models. Mechanisms such as grain boundary mechanics (Ma, Roters, & Raabe, 2006), (Ma, Roters, & Raabe, 2006) or damage initiation (Bieler , et al., 2009) into the constitutive description. Concerning additional deformation mechanisms such as those that occur in TWIP or TRIP steels, extended CPFE formulations have been suggested by (Kalidindi S. R., 2001), (Kalidindi S. R., 1998), (Salem, Kalidindi, & Semiatin, 2005), (Staroselskya & Anand, 2003).

Conclusions

CPFEM is a powerful tool for modelling a wide range of mechanical problems in material sciences and engineering. Its applications vary between various microscopic and macroscopic applications. Tracking its chronological evolution showed that it had to wait until enough evolutions is reached in its two main legs: finite element method and crystal plasticity. Only after enough evolution for each of them and after their mixing together, evolution of new models became possible. Those new models severely needed due to various advances in material science and engineering.

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