Crystal plasticity finite element method application in micro/meso-scaled deep drawing and some related concerns

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Abstract. The crystal plasticity finite element method (CPFEM) has been widely used in the research of micro/meso-scaled deformation of materials. In this talk, the effectiveness of CPFEM in simulating deep drawing processes is highlighted, with a particular focus on modelling complex stress distributions and capturing the effects of material anisotropy and thickness variations. It is found that CPFEM can accurately depict the influence of material properties on formability at these scales. However, the computational cost, the requirement for improved material models to handle deep drawing, and the variety of modelling features for different materials and processes are some serious concerns, which are elucidated in this talk, and the importance of CPFEM in predicting and analysing the precision and efficiency of micro/meso-scaled deep drawing is highlighted.

Keywords: CPFEM; Micro/meso-scaled deep drawing; Material modelling; Computational efficiency.

1 Introduction

Micro/meso-scale cup-shaped components are of great significance in various fields such as microelectronics, robotics, and biomedical engineering. Micro/meso-scale deep drawing (MMDD) deformation is the most widely used and efficient method for producing these components. As component dimensions shrink to the micro/meso-level, they approach the inherent microstructural length scales of materials, such as grain size, leading to pronounced size effects (SE). Material behavior and deformation mechanisms at this scale differ significantly from those in macro-scale processes, making macro-scale deep drawing experience largely inapplicable. Therefore, there is an urgent need to develop and implement novel process optimization methods and material models that account for the unique characteristics of micro/meso-scale deformation. By advancing our understanding and control of these processes, the full potential of MMDD for high-precision manufacturing applications can be unlocked.

In meso/micro-scale metal plastic deformation, the grain SE is a critical factor influencing material behavior. As the size of components decreases to the micro or nano scale, the ratio of grain size to the overall material volume increases, leading to significant changes in mechanical properties. The Hall-Petch relationship illustrates that as grain size decreases, the strength of metals increases. This phenomenon can be attributed to the greater number of grain boundaries in crystalline materials, which serve as obstacles to dislocation movement. When dislocations encounter grain boundaries, they either pile up or change their slip direction, effectively increasing the strength of the material. A critical ratio has been identified for generating the size effect in micro deep drawing processes [1]. All earing effect, anisotropic deformation, and thickness variation has been affected by the grain size [2-4]. These findings highlight the importance of considering grain size effects in the development of new process optimization methods and material models for MMDD deformation.

The Crystal Plasticity Finite Element Method (CPFEM) has emerged as a powerful tool for modelling metal plastic deformation at micro/meso - scales. Unlike traditional FEM, CPFEM incorporates microstructure - level details, such as grain orientation and size, enabling more accurate predictions of material behavior. This method not only considers the actual orientation in polycrystalline materials but also can consider different crystal structure types and slip mechanisms in the plastic deformation of multiphase materials. Compared with traditional finite element simulation, CPFEM can reflect the deformation mechanism of crystal materials and is closer to the realistic plastic deformation process. In one case study, researchers used a three - step progressive micro - forming system to manufacture a hexagonal socket part and compared the experimental results with CPFEM simulations [5]. The focus was on microstructure evolution, deformation load, and product quality. The CPFEM simulations were found to be more reliable than conventional FEM in predicting complex deformation, particularly in microstructure and texture evolution, dimensional accuracy, and irregular geometries. In summary, CPFEM has proven to be a valuable approach for modelling and understanding the

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complexities of metal plastic deformation at micro/meso - scales. Its ability to incorporate microstructural details and capture size - dependent effects makes it an essential tool for advancing the development of MMDD.

Therefore, CPFEM should have a place in the process optimization of MMDD. In the early development of crystal plasticity, Raabe et al. [6-8] and Nakamachi et al. [9, 10] conducted numerous simulations of deep - drawing deformation using CPFEM. They performed crystal plasticity simulations of deep - drawing for BCC steel, aluminium, and alloys. The initial textures came from experimental results, but the FE models were macro - scale, with cup diameters of about 50 - 100 mm. Although these simulations produced some texture evolution data similar to experimental results, they lacked the precision to predict SEs on deformation behavior and product quality. In this review, the focuses are on CPFEM and MMDD. Section 2 presents direct CPFEM applications in MMDD, covering diverse materials and characteristic sizes. Section 3 highlights the advantages of CPFEM in these simulations. Section 4 explores its indirect applications. Section 5 addresses concerns and future prospects. Section5 summarizes the key points.

2 Direct applications of CPFEM in MMDD

Over the past decade, numerous studies have focused on SE in MMDD, aiming to enhance forming limits and improve quality. This review emphasizes research on the feasibility of producing micro - parts with high height-to-outer - diameter ratios through single micro - forming stages. Table 1 presents representative literature on direct CPFEM applications in MMDD. "Direct application" means using CPFEM to simulate the whole process of MMDD, considering texture evolution and overall deformation, including crystal orientation distribution, grain size and morphology changes, thickness variation, earing, and other defects from heterogeneous deformation.

Table 1. Some examples for direct applications of the CPFEM in MMDD. (t-sheet thickness; D-cup diameter; d-average grain size.)

Material	t/mm	D/mm	d/μm	Ref.
Pure Cu	0.05-0.1	1-2	30-100	Zhang and Dong [11]
TWIP Steel	0.1-0.2	1.7	30-50	Guo et al. [12]
SS 430	0.05	0.95	14-25	Zhao et al. [13]
TRIP Steel	0.12-0.25	3-10	23-28	Zhang et al. [14]
ASS 304	0.02	0.9	7-19	Zhao et al. [15]

First, Zhang and Dong [11] simulated MMDD of pure copper sheets using a dislocation - density - based crystal plasticity model. Their simulation results for height distribution and load curves were consistent with experimental data. Then, Guo et al. [12] and Zhao et al. [13] respectively studied the effects of grain size and sheet thickness on the deformation behavior of TWIP steel and SS 430 in MMDD. They focused on slip system activation and twinning effects. Zhang et al. [14] mainly focused on the deformation behaviours of different phases in TRIP steel in MMDD. Zhao et al. [15] particularly examined the grain SEs on the surface quality of MMDD products. Fig. 1 shows the CPFEM simulation results of MMDD, including the grain morphologies, stress and strain maps.

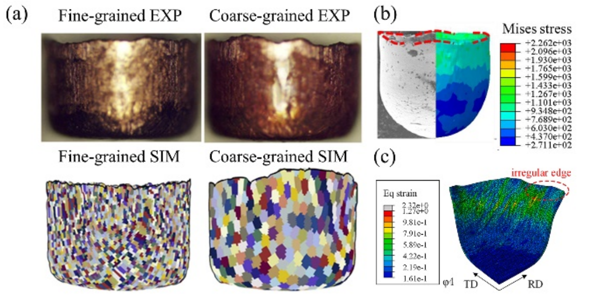

Fig. 1. Micro/meso-scaled cups formed by MMDD through experiments and simulations. (a) Comparison between the experimental products and the simulated grain morphologies. [11] (b) The stress map for a 4-earing type micro cup with the ratio of *d* to *t* of 0.25. [12] (c) Strain map of the simulation results of a TRIP steel cup. [14]

2.1 Modelling of MMDD

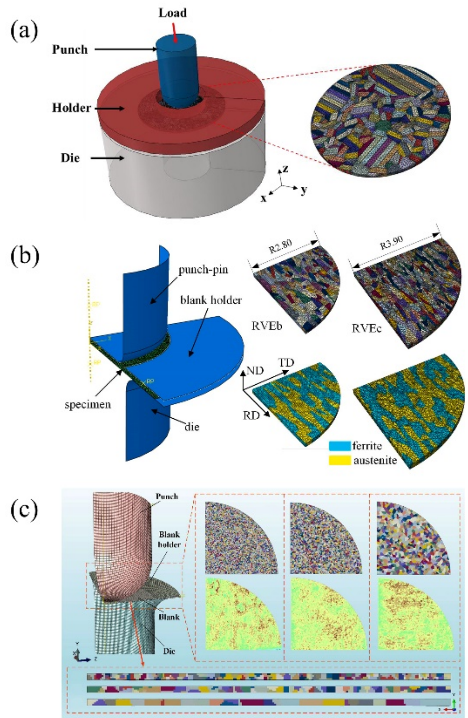

Fig. 2. Finite element model of MMDD. (a) Holistic model [12], (b) quarter two-phases model [14], and (c) quarter models for different grain sizes [15].

The modelling process of CPFEM differs from traditional FEM in several aspects. Traditional FEM usually treats materials as homogeneous and isotropic, focusing on macroscopic mechanical responses and ignoring microstructural details. In contrast, CPFEM incorporates microstructure-level details, such as grain orientation, size, and morphology, into the finite element model, enabling more accurate predictions of material behavior. Fig. 2 shows in detail the modelling of MMDD in CPFEM.

In CPFEM, each grain or a group of grains with similar orientations is considered as a separate unit, and their interactions are modelled based on crystal plasticity theory. This method not only considers the actual orientation in polycrystalline materials but also can consider different crystal structure types and slip mechanisms in the plastic deformation of multiphase materials. To study the unique earing and thickness changes in deep - drawn parts, 3D material modelling is essential. In related studies, both 3D hexahedral and tetrahedral elements were used. As shown in Fig. 2(c), the number of grains in the thickness direction is small, indicating the potential impact of grain size on simulation results. For 3D complex deformation simulations, directly converting material characterization results into models is rarely used due to two main reasons: (a) Current microstructure characterization methods like EBSD and TEM are 2D, and accurately converting them to 3D models remains challenging; (b) Directly converting EBSD data to models requires a mesh size smaller than or equal to the step size, significantly increasing the number of meshes and the already high cost of CPFEM simulations. Therefore, in current 3D complex deformation CPFEM simulations, most studies use the Voronoi method to describe polycrystalline aggregates to model grains with desired shape and size, and then fill in material characterization data such as crystal orientation.

2.2 Crystal plasticity constitutive models

Currently, CPFEM for part processing is mostly based on phenomenological methods. In crystal plasticity modelling, it is generally assumed that there exists an intermediate configuration between the initial and current configurations, which involves pure plastic deformation and elastic unloading, as illustrated in Fig. 3. This assumption is crucial for accurately capturing the material's behavior during processes like deep drawing, where plastic deformation and elastic recovery play significant roles. The total deformation gradient $\boldsymbol{F}$, imparted upon a crystalline material by means of crystal slip or twinning, can be decomposed into two constituent parts: the plastic deformation gradient $\boldsymbol{F}^p$ (from slip or deformation twinning) and the elastic deformation gradient $\boldsymbol{F}^e$ (from the reversible stretching and rotation of the crystal lattice):

$$\boldsymbol{F} = \boldsymbol{F}^e \cdot \boldsymbol{F}^p \tag{1}$$

The instantaneous velocity gradient $\boldsymbol{L}$ is given by:

$$\boldsymbol{L} = \dot{\boldsymbol{F}} \cdot \boldsymbol{F}^{-1} = \dot{\boldsymbol{F}}^e \cdot \boldsymbol{F}^{e\,-1} + \boldsymbol{F}^e \cdot \dot{\boldsymbol{F}}^p \cdot \boldsymbol{F}^{p\,-1} \cdot \boldsymbol{F}^{e\,-1} \tag{2}$$
$$\boldsymbol{L}^p = \dot{\boldsymbol{F}}^p \cdot \boldsymbol{F}^{p\,-1} \tag{3}$$

$\boldsymbol{L}^p$ (plastic distortion rate) can be expressed by introducing the Schmid law:

$$\boldsymbol{L}^p = \sum_\alpha \dot{\gamma}^\alpha (\boldsymbol{m}_0^\alpha \otimes \boldsymbol{n}_0^\alpha) \tag{4}$$

where $\boldsymbol{m}_0^\alpha \otimes \boldsymbol{n}_0^\alpha$ is the Schmid factor, and $\dot{\gamma}^\alpha$ is the plastic shearing rate of the slip or twinning system α. Eqs. (1)-(4) form the fundamental part of the CPFEM model that is widely used. The latter part varies significantly depending on the material and evolution method. In the study by Zhang and Dong [11], a dislocation - density - based method was used in the evolution equations for shear rate and hardening rule, incorporating concepts of activation energy and volume. In contrast, Guo et al. [12], when studying TWIP steel, which exhibits substantial deformation twinning, considered the self - hardening, cross - hardening of twin systems, and their hardening relationship with the slip systems. The most commonly used formulation in the current CPFEM applications is to consider only the self-hardening and cross-hardening of the slip system, but it has the disadvantage of only being able to describe the material state in terms of the critical decomposition shear stress.

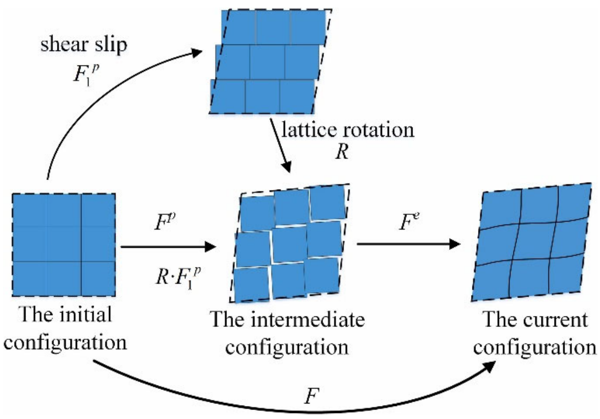

Fig. 3. Multiplicative decomposition of deformation gradient. [16]

3 Advantages of CPFEM in MMDD simulation

In this section, the superiority of CPFEM in MMDD simulations is presented by comparing the simulation results. The analysis focuses on common MMDD issues: thickness non-uniformity and surface quality, anisotropic deformation and earing, and microstructural and texture evolution.

3.1 Thickness non-uniformity and surface quality

In MMDD, thickness non - uniformity is critical as the cup bottom, the main load - bearing area, thins significantly, while the maximum thickness relates to wrinkling and the minimum to fracture. In MMDD, uneven deformation causes irregular product shapes. Fig. 4(a) compares the numerical and experimental thickness distribution results, showing good agreement, with thinning at the bottom and thickening at the flange. The thinnest area is the nose radius or transition area, due to tension from friction on side wall and punch pressure on the bottom. Fig. 4(b) shows grain SE on thickness distribution. As grain size increases, thickness fluctuation and strain localization - induced necking rise.

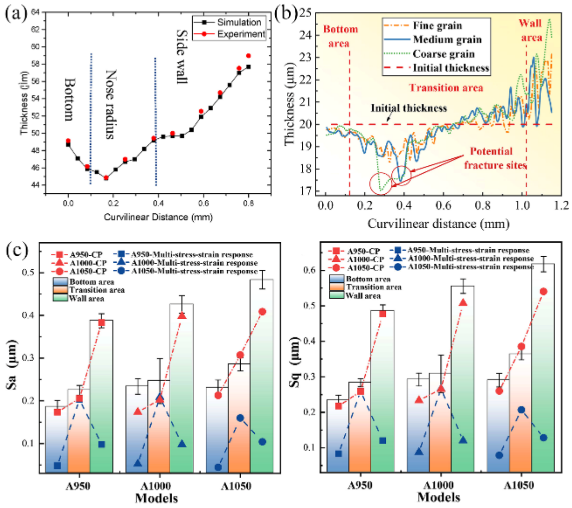

Fig. 4. CPFEM simulation and experimental results of thickness distribution of drawn cups: (a) SS430 [13] and (b) SS304 [15]. (c) Surface roughness of the micro cups [15].

Fig. 4(c) compares the surface roughness in different regions from CPFEM simulations and experiments. The overall trend in surface roughness from the CPFEM model aligns with experimental results, unlike traditional finite element results that show significant discrepancies. Thus, the CPFEM model has a clear advantage in surface roughness analysis. Moreover, the results indicate that as grain size increases, so does the roughness of micro - parts, which may be related to the microstructure.

3.2 Anisotropic deformation and earing

In MMDD, earing is a common defect where the flange of the drawn part becomes wavy or forms ears due to material anisotropy and uneven deformation, as shown in Fig. 1. This occurs because the material's resistance to deformation varies with direction, often influenced by its crystallographic texture and microstructure. The earing in MMDD is significant for several reasons. Firstly, it affects the dimensional accuracy and aesthetic quality of the final product. Secondly, it can influence the mechanical properties and performance of the part, particularly in applications where precise geometry and uniform thickness are critical.

In order to clarify the effect of SE on the ear-like profile, Guo et al. [12] utilized different λ values in the size-dependent CPFEM simulation. As shown in Figure 5 (a, b), the simulated and experimental ear-like features with size scaling factors of 1/2 and 1/4 are compared. When λ=1/2 and λ=1/4, different ear-like types and numbers appear, including two 0°/180° and four 0°/90°. For randomly distributed crystal orientations, the different ear-like features under different size scaling factors can be attributed to the grain and geometric size. With the increasing trend of λ, that is, the grain size increases and the geometric size decreases, the microstructure of the sample is equivalent to the single crystal case in extreme cases. Obvious planar anisotropy occurs, resulting in obvious ear-like profiles.

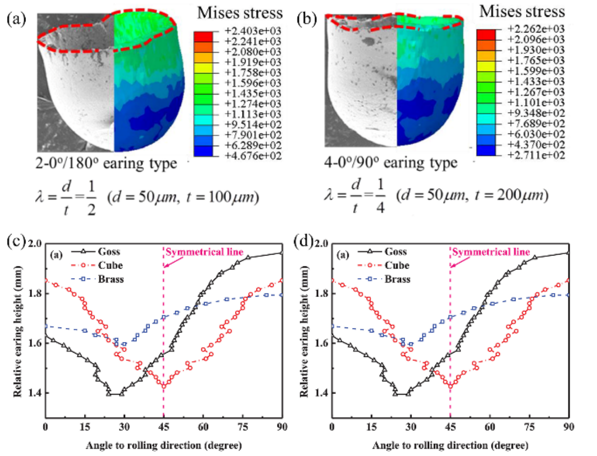

Fig. 5. Comparisons of the experimental and simulated earing profiles with the size scaling factor 1/2 (a) and 1/4. Earing characteristics of samples with different initial grain orientations: (c) cup height and (d) earing rate. [12]

3.3 Microstructure and texture evolution

In MMDD, varying grain orientations activate different slip systems, leading to diverse deformation behaviours under the same strain conditions. The deformation is mainly orientation - dependent due to the consistent force direction. For instance, Zhao et al. [15] analysed the stress - strain modes and morphology of differently textured micro – parts, as shown in Fig. 6. The strain frequency distribution of each slip system model shows that differently activated slip systems during deformation lead to varied strain distributions. Comparing Fig. 7(a-c), Goss - oriented grains experience larger strains across more slip systems than Brass and {112}〈110〉 - oriented ones, indicating greater deformation. The strain magnitude varies across slip systems due to different activation difficulties for the same force direction.

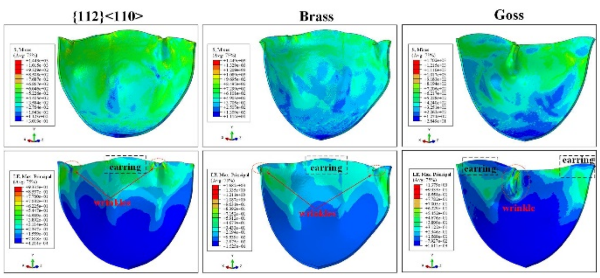

Fig. 6. Von Mises stress (1st line) and logarithmic strain (2nd line) distribution of models with different texture. [15]

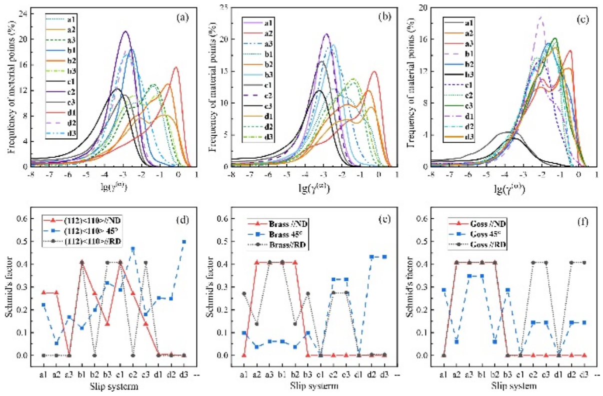

Fig. 7. The logarithmic value of the strain in each slip system (1st line) and the Schmid's factors along different directions (2nd line): (a, d) {112} 〈110〉, (b, e) Brass, (c, f) Goss.[15]

4 Indirect applications of CPFEM in MMDD

The "indirect application" of CPFEM in MMDD differs from direct simulation of the manufacturing process. Instead, it's used in a microstructure - based computational framework that accounts for evolving textures. Here, CPFEM and phenomenological constitutive models interact to update textures and plastic anisotropy at grain and engineering length scales. As shown in Fig. 8, CPFEM first performs a simple tension simulation on a representative volume element (RVE) to determine the material's yield surface, which is related to texture and crystal orientation. This yield surface is then used in traditional FEM for MMDD simulation. In this review the indirect applications of CPFEM in MMDD are mentioned but not delve into details. For in - depth information, please refer to relevant literature [17-20].

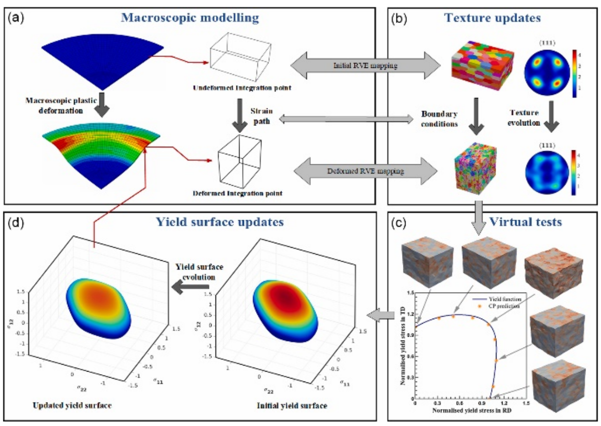

Fig. 8. Schematics of the indirect application of CPFEM in MMDD. The CPFEM is used to validate the yield surface. [17]

5 Related concerns and future

The extensive use of CPFEM in MMDD and the promising results obtained have demonstrated its practicality. However, it's crucial to have a comprehensive understanding of this method. The following points are some related concerns:

5.1 Balance Between Efficiency and Accuracy

CPFEM's strength in modeling microstructure - induced deformation comes at a computational cost. Researchers must balance model complexity and computational efficiency, especially for industrial applications. Simplified CPFEM models or high - performance computing resources could enhance efficiency without sacrificing accuracy. The high computational cost of CPFEM is primarily due to the need to run independent microscopic models at each macroscopic integration point. This significantly increases the computational workload. Additionally, the use of uniformly structured meshes in CPFEM simulations can further increase computational costs. For example, in diffused interface CPFEM, uniform meshes can lead to unnecessary computations in regions where stress and strain gradients are small. To address this, biased mesh generation algorithms have been developed to reduce computational costs while maintaining accuracy. These algorithms allow for coarser meshes in regions with low gradients and finer meshes near grain boundaries where gradients are high. The use of non - conformal elements in mesh size transition regions also helps maintain computational efficiency without compromising accuracy. The development and implementation of such algorithms are crucial for making CPFEM more practical for industrial applications.

5.2 Practicality of CPFEM Simulation Results

CPFEM simulations offer detailed insights into material behavior at the micro - scale, such as grain - level deformation and texture evolution. However, translating these into practical process optimizations or quality improvements remains challenging. One of the main challenges is the complexity of the models themselves. CPFEM involves complex constitutive and internal variable details of the process history and environmental factors into the structure–property relations, leading to strong nonlinearity of the system. This complicates the derivation of sensitivities, which are essential for understanding the effect of each material parameter. Another challenge is the need for extensive experimental validation. While CPFEM can predict surface roughness changes due to grain orientation, for instance, these predictions must be validated against real - world manufacturing results to ensure reliability. This validation process is time - consuming and requires careful experimental design. Additionally, the integration of CPFEM results into existing manufacturing workflows is non - trivial. Manufacturing processes often rely on macro - scale models for process control and optimization. Bridging the gap between micro - scale CPFEM results and macro - scale process parameters require developing new protocols and tools.

5.3 Adaptability and Extensibility of CPFEM in MMDD

CPFEM has been successfully applied to various materials and processes, but its adaptability to new materials or complex processes needs enhancement. Additionally, integrating CPFEM with other advanced modelling techniques, such as the cohesive zone model (CZM), is crucial for fully capturing deformation and failure mechanisms in MMDD. In progressive micro - forming, CPFEM has shown its ability to provide physical insights into how grain size affects the interaction between crystal slip and mechanical twinning in complex micro - forming. CPFEM was found to be more reliable than conventional FEM in predicting complex deformation, especially in microstructure and texture evolution, dimensional accuracy, and irregular geometries. Future research should focus on improving the efficiency and accuracy of CPFEM simulations for MMDD. This could involve developing simplified CPFEM models or using high - performance computing resources. More experimental validation is needed to ensure the reliability of CPFEM predictions. The development of standardized protocols for material characterization and model calibration would also enhance the applicability of CPFEM in industrial settings. Finally, combining CPFEM with other advanced modelling techniques, such as damage and fracture model (CZM, GTN model, etc), recrystallization (phase field method and cellular automata), could provide a more comprehensive understanding of the complex deformation behaviours in MMDD processes.

6 Conclusions

This review comprehensively examines the application of CPFEM in MMDD, summarizing its achievements, raising some concerns and offering future prospects.

The significance of SEs in MMDD and how CPFEM accurately captures microstructure-induced heterogeneous deformation and texture evolution have been explored. By incorporating microstructural details, CPFEM provides deeper insights into material behavior during MMDD than traditional FEM, enhancing process optimization and product quality.

However, challenges remain in applying CPFEM to MMDD. The high computational cost and complexity of models pose obstacles for industrial use. Ensuring the reliability of CPFEM predictions requires extensive experimental validation, which is time-consuming and demands careful experimental design. Additionally, interpreting CPFEM results and integrating them into existing manufacturing workflows need specialized knowledge and new protocols.

Future research should focus on improving CPFEM's computational efficiency and accuracy. This could involve developing simplified models, leveraging high-performance computing resources, and creating standardized protocols for material characterization and model calibration. Integrating CPFEM with other advanced modelling techniques could also provide a more comprehensive understanding of the complex deformation behaviours in MMDD processes.

In conclusion, CPFEM has shown great potential in modelling and understanding the complexities of metal plastic deformation at micro/meso-scales. Addressing the current challenges and advancing CPFEM capabilities will further enhance its applicability and effectiveness in MMDD, paving the way for more innovative and high-precision manufacturing processes.

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