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# Study of microstructural grain and geometric size effects on plastic heterogeneities at grain-level by using crystal plasticity modeling with high-fidelity representative microstructures

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In-depth understanding of plastic heterogeneities at grain-level and local deformation behaviors is pivotal in exploring the mechanical response and fracture mechanism of thin metal sheets in micro-scale deformation. This work employs a state-of-the-art crystal plasticity spectral method in conjunction with comparable high-fidelity microstructures to study the coupling effect of micro-mechanical (intrinsic) heterogeneities introduced by grain size, morphology, orientation, and inter-granular interaction, as well as macro-mechanical (extrinsic) heterogeneities imposed by geometrical features (*i.e.*, thickness and free surface). The study reveals that the extrinsic and intrinsic factors influence the plastic heterogeneity and fracture failure of metal foils via affecting: (i) the strain and stress fluctuations at grain-level, which are directly related to the fracture morphology observed experimentally; (ii) the morphology of local shear bands which accounts for the transformation of fracture modes with the decrease of the ratio ($\lambda$) of thickness to grain size; and (iii) statistical characteristics of plastic heterogeneities which interpret the sharp reduction of the fracture toughness with the decrease of $\lambda$. Moreover, the research further presents some findings about the influence of the examined factors on the stress and strain heterogeneities, lattice rotation, slip system activation, and the surface roughness of the material. This work therefore provides a well-rounded exploration of micro-scale plasticity of metal foils at grain-level, and serves as a physically motivated basis for the development and modeling of fracture and failure of metal polycrystals in micro-forming process.


## 1. Introduction

The rapid development of miniaturized devices and products places high demands on micro-components and micro-parts with thickness ranging from tens to hundreds of microns. Due to their suitability for mass and low-cost production, micro-forming operations are a promising method for manufacturing the micro-parts (Fu and Chan, 2013). However, challenges

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related to the feature size of micro-parts and the microstructural size of materials, and various size effects resulted from the complicated interaction between geometrical constraints and material microstructure (Geers et al., 2006; Kraft et al., 2010; Fu et al., 2016), render the well-established know-how of conventional metal forming invalid or inaccurate in micro-forming. Numerous works have been carried out to assess the influence of sample size (*e.g.,* thickness $t$) and grain size ($d$) on marco-scale mechanical manifestations such as flow stress, springback angles, work hardening, forming limit, fracture toughness, *etc.* (Chan and Fu, 2011; Yang and Lu, 2013; Keller et al., 2012; Liu et al., 2012; Wang et al., 2016). While the grain-scale mechanics and heterogeneity resulted from the coupling effect of material microstructures and geometry features (*e.g.,* thickness and free surfaces) require in-depth understanding and further investigation, as they are crucial for the plastic instability and failure of metal polycrysals in micro-forming.

Fu and Chan (2011) performed the micro-tensile test of copper foils, and found that the fracture stress, the fracture strain, and the number of micro-voids decrease with the ratio ($\lambda$) of thickness to grain size. Micro-tension of copper foils carried out by Chauhan and Bastawros (2013) reveals that the competing influence between free surface effects and inter-granular interactions accounts for the reduction of strength and ductility with the decrease of thickness. The micro-tensile tests of pure copper foils performed by Yang and Lu (2013) and Meng and Fu (2015) show that the reduction of $\lambda$ changes the fracture mode from normal tensile failure to pure shear failure. It was attributed to the competition between the dislocation activities in interior grains and surface grains (Yang and Lu, 2013) and the reduction of activated slip systems with the decrease of $\lambda$ (Meng and Fu, 2015), respectively. However, neither experimental nor simulation evidences were provided for these explanations. A premature rupture was also observed in the micro-tensile tests of stainless-steel foils, *i.e.,* the foils fractured without obvious diffuse necking (Pham et al., 2015). They explained it based on the evolution of surface roughness and material heterogeneity in the thickness and suggested further works to clarify the mechanism.

Metal polycrystals are inherently heterogeneous at grain-level. Microstructural heterogeneities makes both strain and stress fields inhomogeneous from the beginning of deformation, and their evolution naturally results in strain localizations, local shear bands, distinct stress concentrations, and nucleation of damage, which further affect the fracture and failure behaviors and surface roughness of metal foils (Raabe et al., 2001; Yoshida, 2016). Thus, the sample size, free surface, grain size, and crystallographic orientation simultaneously affect the plastic heterogeneity and mechanical response of metal polycrystals, and their coupling effects mainly account for the unusual phenomena observed in micro-scale plastic deformation. These effects are more pronounced in the case of thin metal sheets because the limited number of grains in the thickness renders strong interactions between geometrical and microstructural size effects. Grain-scale heterogeneities thus could cause loss of structural stability in miniaturized devices whereas they may not have in bulk components (Raabe et al., 2001). For micro-scale plastic deformation, therefore, the inter-granular and intra-granular inhomogeneous plastic behaviors should be considered extensively, and grain-level investigations beyond the continuum scale assumptions are indispensable for explaining the above reported phenomena.

Experimentally, many novel approaches were developed to explore the micro-scale plastic behavior and to track the evolution of inhomogeneous strain fields throughout a plastic deformation process, such as in-situ tests in union with SEM, EBSD, and digit image correlation (DIC) for measuring the surface deformation (Kadkhodapour et al., 2011; Tasan et al., 2014, 2015) and 3D X-ray diffraction for measuring subsurface lattice rotations and stress heterogeneities (Wang et al., 2010b; Abdolvand et al., 2015a). Sachtleber et al. (2002) used photogrametry in conjunction with microtexture experimentation to investigate the grain-scale strain heterogeneity of aluminum polycrystals during plane compression, and found that strain patterning is strongly determined by the orientation of individual grains. Guery et al. (2016) studied the plastic behavior of 316LN austenitic stainless steels by using in-situ mechanical tests and DIC jointly. It is observed that the strain fields are markedly heterogeneous with numerous shear bands either aligned with or interrupted by grain boundaries (GBs). High quality patterns, high magnification imaging systems, and careful sample preparation, nevertheless, are the prerequisite for evaluating the heterogeneity of micro-mechanical responses, and the variation of these prerequisites significantly affects the detected results (Joo et al., 2013). DIC experiments conducted by Efstathiou et al. (2010), for example, show that grain-scale deformation patterns, *i.e.,* the inclined slip bands near GBs and GB triple junctions (GBTJs), can only be detected by their DIC experiments with the highest optical magnification.

These progressive experimental techniques undoubtedly contribute a lot to the exploration of plastic heterogeneities. However, due to the limited stress and strain partition at the micro-/submicro-scales as well as the complexities resulted from heterogeneous grain morphology, crystallographic orientation, and inter-granular interaction, it is hard to experimentally get a comprehensive examination of micro-scale plastic behaviors and grain-level heterogeneities, especially for metal forming which generally involves large deformation. Moreover, the overlap of macro-mechanical (extrinsic) heterogeneities imposed by geometrical conditions on one hand and micro-mechanical (intrinsic) heterogeneities introduced by grain size, grain interaction, and grain boundaries on the other hand, requires the separation of the extrinsic and intrinsic effects for a genuine grain-level heterogeneity research (Raabe et al., 2001). Such separation is yet challenging for both experiments and numerical simulations.

To fully understand the grain-scale plastic behavior and heterogeneity of metal polycrystals, crystal plasticity (CP) based simulation techniques are particularly well suitable for remedying experimental approaches. CP based modeling is adept at describing the mechanical response of individual grains and naturally connecting macroscopic mechanical behaviors with microstructural origins (Roters et al., 2010, 2013). It is thus frequently used to predict texture evolution, earing, and surface roughening (Raabe et al., 2007; Tikhovskiy et al., 2008; Jia et al., 2012b), to study mechanical anisotropy, grain interactions, and GB mechanics (Sachtleber et al., 2002; Zaefferer et al., 2003; Su et al., 2016), and to simulate martensite transformation

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