

Strain Statistics Evolution in Crystalline Material through Statistical Analysis

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Abstract. The deformation in crystalline materials is highly heterogeneous. Many different types of distributions are employed to describe the stresses and strains statistics in different crystalline materials. The objective of the current study is to find a proper distribution to describe the strain statistics during deformation evolution in crystalline materials with different crystal type. Both experiment and CPFEM simulation were carried out at the same time. For the experimental data, the local strain distribution from different crystalline materials with BCC, HCP, FCC crystals under tensile loading can be well described by generalized extreme value fit. Additionally, we use the simulation data from nickel-base superalloy as an example to justify this result, and this also indicates that both plastic and elastic conform to the generalized extreme value fit for all deformation stage ranging from 0% to 30% strain.

Keywords: Crystalline Material; Statistical Analysis; CPFEM Simulation.

1. Introduction

Crystal is a solid material that has orderly arrangements of the atoms, such as metals and salts. This kind of material is widely used in our lives. For instance, some wear-resisting crystal materials, like ceramics and stainless steel, are mainly used in infrastructure and aircraft manufacturing. Moreover, one of the hardest crystals — the silicon element, is also a non-metallic element with a crystal structure, which is highly connected to people's lives.

The local deformation of crystalline materials is relatively heterogeneous. The total deformation in crystals can be divided into the elastic part and the plastic part. When acting a force onto a crystal material, it will first be linearly stretched, and until a particular force, the extension will then not be linear. Linear deformation corresponds to elastic part, while nonlinear deformation represents the plastic part. At the microscopic level of the crystal deformation, the atoms will be stretched in elastic stage during tension and compression loading and they will return to their original state if the force is removed. However, the plastic deformation occurs by crystal slip (rearrangement of atoms), the atomic bonds will be broken and reconnected. There are three basic concepts in plastic deformation. Firstly, crystal slip often occurs in particular slip planes, which are surfaces for particles being stretched. Secondly, atoms will be easier to slide in specific directions than in other directions. The combination of slip planes and slip direction are called slip system. Usually, the slip plane will be the most densely packed plane in the crystal, and the slip direction will be on the slip plane along the denser atoms. Different factors affect the deformation mechanism of the crystal, including the crystal structure, the size of the atoms, the bond between the atoms (covalent, metallic, or ionic), and the type of material.

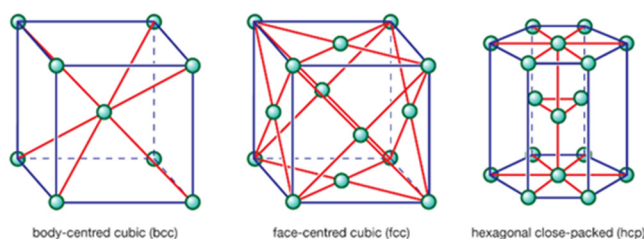


Figure 1. The particular crystal structure for three cubic crystals.

Figure 1 illustrates the crystal structure of three cubic materials, namely face-centered cubic (FCC), body-centered cubic (BCC) and hexagonal closest packed (HCP). BCC's main advantage is that it can exhibit high strength over a wide temperature range and in a significant strain. There are many strong planes in these crystals. However, in FCC, the slip surfaces (firm surfaces) usually do not change. For HCP, it is a minor natural protein. This crystal is the most basic structural feature of their internal atoms, ions, and molecules arranged in space as a three-dimensional periodic regular arrangement. Any crystal can always find a set of base vectors corresponding to three-dimensional periodicity and corresponding unit cells.

In this research, we will comprehensively study the strain distribution evolution in deformation processing by analyzing the strain mapping of various crystal materials published in literature, and mathematical modeling of the crystal deformation process using the crystal plasticity finite element method. The investigation results, together with the simulation results, will provide a more reliable statistical distribution result.

2. Literature Review

There are three main scales of plastic deformation in terms of its characteristic length scale and its controlling microstructure features: microscale, mesoscale, and macroscale. For the microscale, since plastic deformation is characterized by dislocation motion, dislocation-dislocation interactions, and dislocation interactions with other crystal defects, and these all are controlled by the crystal structure and defect distribution, both the strain and stress can only be obtained by averaging atomic-scale properties over a certain region. The plastic deformation on the mesoscale (grain scale) is characterized by strain and stress inhomogeneity that appears within and between grains. The microstructural characteristics on the mesoscale, including grain size and orientation, phase properties, dislocation density, and their distributions, are what regulate it. On the macroscale, the plastic deformation exhibits strain and stress inhomogeneity between various portions of the sample on the macroscale (sample scale). The sample shape, loading circumstances, and averaged material characteristics—with the impacts of microstructural heterogeneity removed—are the regulating elements of plastic deformation at this scale since the entire sample is conceived of as a continuous medium with homogenous qualities [1].

Here the research mainly concentrates on the distribution of local (microscale) plastic deformation in crystals. When studying the relationship between microstructure and mechanical properties, the relevance of a microstructure's mesoscopic characteristics, dislocation density, and distributions, as well as plastic deformation, is frequently neglected. The above microstructural properties are often averaged when investigating the mechanical behaviors of crystals, which will be likely to introduce further uncertainty in the strain distribution result. For example, the exceptional features of gradient-grained metals cannot be predicted by the average grain size alone. The typical volume-averaging technique cannot forecast the greater strength present in the scenario where the martensite is continuously distributed than that present in the discretely distributed case in dual phase (DP) steels with the same average volume percentage of martensite. This averaging method's failure results from a distinct distribution of mesoscopic strain and stress caused by the variation of grain size [2].

As a result, as the main characteristics of mesoscopic strain distribution are strain inhomogeneity within the grain and between the grains and phases, with extreme manifestations exhibited as deformation bands or shear bands. While a considerable number of studies has concentrated on the averaged macroscopic properties, comparatively less attention has been paid to the statistical distributions of the local microscopic behaviour within strain/stress fields. Furthermore, failure in polycrystalline alloys frequently originate in highly localized fields where intergranular and intragranular strain and stress dominate. A pointwise experimental evaluation of strain field with material microstructure remain rather costly and time-consuming, whereas a statistical description of strains and stresses may improve the understanding of the deformation process. Local plastic slip distributions have been widely studied and it is well known that they follow an exponential

distribution within the volume of interest [1,3,4]. Tang et al. employed microscale digital image correlation (DIC) and crystal plasticity finite element methods (CPFEM) to investigate the distribution of local strain [1]. They reported the distribution of total strain follows a lognormal distribution. While Tang's research mainly focused on the total strain, they did not study the distribution of local elastic and plastic strains separately. Chen et al. decomposed the total strain into elastic and plastic components and discovered that the elastic strain obeys a normal distribution while plastic strain conforms to a lognormal distribution [4]. Most of the reported literature only investigated the strain statistics in a particular material and within a limited range of strain level. More polycrystalline materials and larger strain loading level should be studied to improve the understanding the spatial inhomogeneity of strain.

3. Methodology

Statistics analysis is carried out in this research using three types of distribution, including normal distributions, lognormal distribution and Gumbel distribution. Firstly, experimental data from different materials were collected and analyzed for polycrystalline materials with FCC, BCC and HCP crystal structure. CPFEM simulation is carried out by using the nickel-base superalloy nominated Haynes 282, which is widely used in aerospace. Since this superalloy will perform its mechanical properties better in high temperature and pressure than other alloy, this material is suitable for this experiment when studying its strain.

3.1 Statistical Distribution

The probability density function of normal distribution is given by Equation (1), where μ and σ are the mean and standard deviation of the variable x respectively. As shown in Figure 2, the peak of normal distribution always locates in the middle of the graph and represent the mean of the data. The distribution is symmetric and the mean value is the axis of symmetry.

$$f(x|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} \quad (1)$$

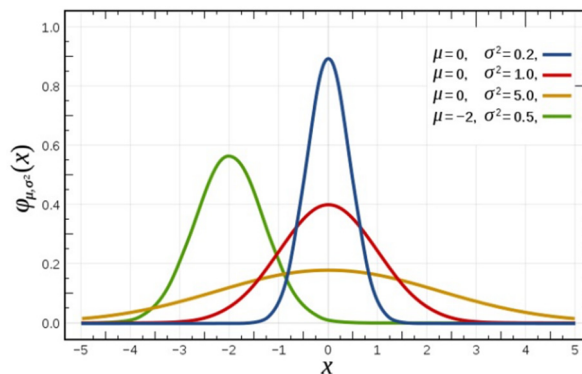


Figure 2. Illustration for normal distribution with different parameters

The probability density function of lognormal distribution is defined by Equation (2), showing that the logarithm of a random variable x obeys the rule of normal distribution. The M and S in Equation (2) are respectively the mean value and standard deviation of the variable $\ln x$. In a limited range, this kind of distribution has the similarity with normal distribution but with a long tail when the independent variable x become large.

$$f(x|M, S) = \frac{1}{xS\sqrt{2\pi}} \exp\left\{-\frac{(\ln x - M)^2}{2S^2}\right\} \quad (2)$$

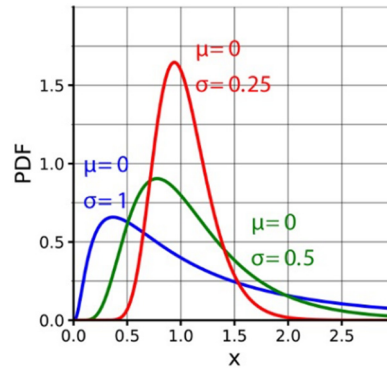


Figure 3. Illustration for lognormal distribution with different parameters

The probability density function of generalized extreme value distribution is calculated using Equation (3), where μ and σ are the location parameter and scale parameter respectively. The shape parameter $k \neq 0$. Although generalized extreme value distribution is often used in oceanography, hydrology and meteorology, there would take place some new discoveries when adding to this strain evolution research. When $k = 0$, the generalized extreme value distribution will reduce to Gumbel distribution, as calculated in Equation (4).

$$y = f(x|k, \mu, \sigma) = \left(\frac{1}{\sigma}\right) \exp \left(- \left(1 + k \frac{(x-\mu)}{\sigma} \right)^{-\frac{1}{k}} \right) \left(1 + k \frac{(x-\mu)}{\sigma} \right)^{-1-\frac{1}{k}} \quad (3)$$

$$g(x|\mu, \sigma) = A_2 \exp \left[-\exp \left[-\frac{(x-\mu)}{\sigma} \right] - \frac{(x-\mu)}{\sigma} \right] \quad (4)$$

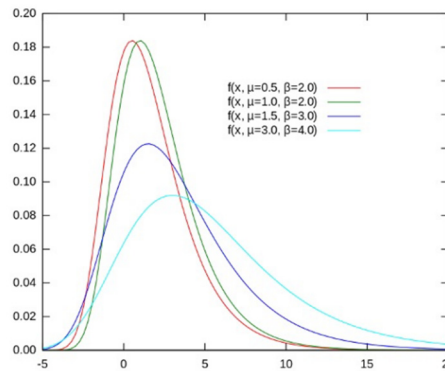


Figure 4. Illustration for Gumbel distribution with different parameters

3.2 The Simulation Procedure for CPFEM Model

The CPFEM model was another technique which was implemented using phenomenological crystal plasticity constitutive equations developed by Manonukul & Dunne [5]. It was further extended to account for elastic anisotropy and to allow three-dimensional modelling for alloys with various crystal structures [6,7]. To calibrate the material parameters in CPFEM, the overall response of a representative volume element (RVE) with 1500 grains during tensile loading was fitted to the experimental stress-strain curve for a nickel-based superalloy nominated Haynes 282. Periodic microstructure and periodic boundary were employed in the RVE shown in Figure 5 (a). Optimal values of material parameters were determined by fitting the macroscopic and mesoscopic response of RVE to the experimental stress-strain curve and neutron diffraction measurement obtained by Jaladurgam et al. [8]. Figure 5 (b) compares the predicted stress-strain curve with the experiment curve and shows that excellent agreement was achieved.

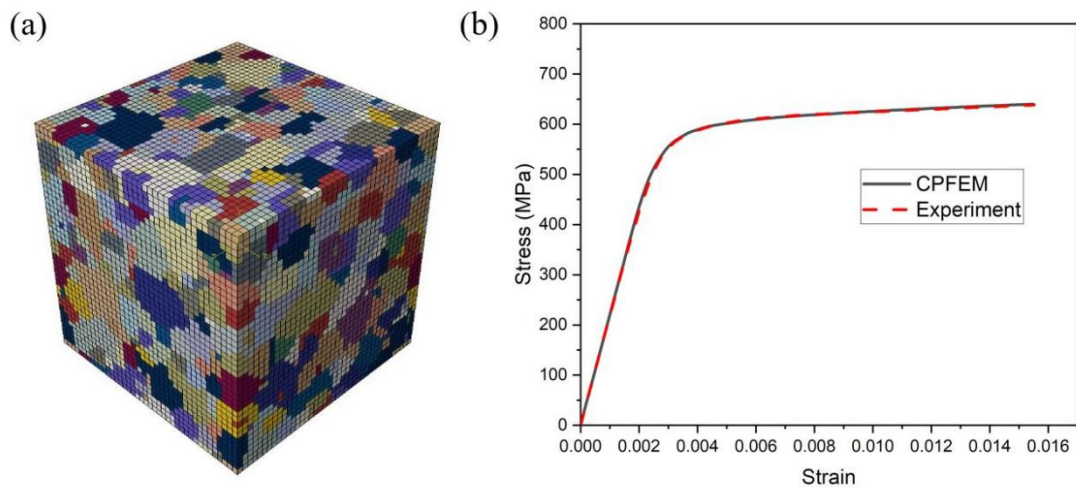
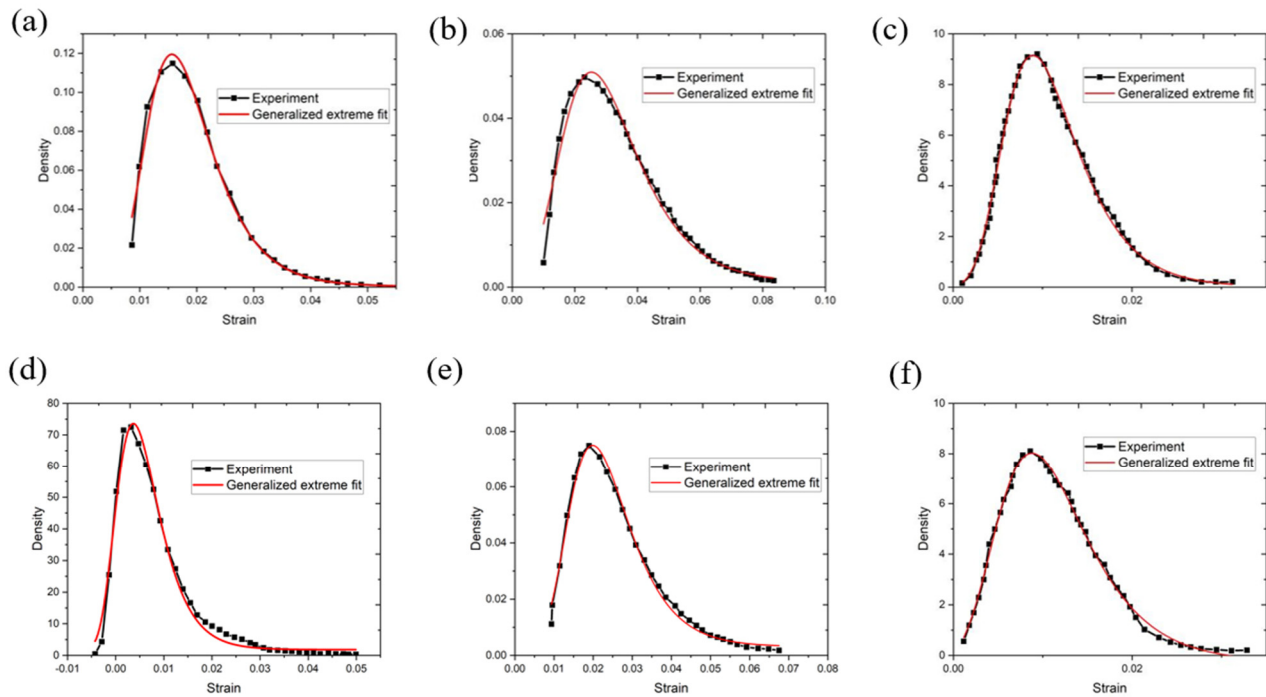


Figure 5. (a) The microstructure of the RVE used to calibrate the materials parameters (different colours indicate different grains). (b) The tensile stress-strain curve obtained from CPFEM prediction and experimental data.

4. Results



- a) RR1000 nickel-based superalloy local strain distribution
- b) RR1000 nickel-based superalloy local strain distribution
- c) 26mm thickness pure titanium plate local strain distribution
- d) Manufactured 316L stainless steel local strain distribution
- e) RR1000 nickel-based superalloy local strain distribution
- f) 26mm thickness pure titanium plate local strain distribution

Figure 6. The local strain distribution from different materials under tensile loading, and fitted with generalized extreme value fit

Figure 6 illustrates the local strain statistics in different materials obtained from the literature. Table 1 lists the researched material in Figure 6 and its corresponding crystal structure. Tensile loading was applied to all the materials, and the loading were stopped when the total strain reached 1% ~3%. It is clear that all the local strain distribution can be well described by generalized extreme fit for all and materials and different loading stage. However, the total strains in Figure 6 are all under 3%, there is little experimental report of strain distribution when the total strain is above 3%. In the following section, CPFEM simulation is used to study the local strain distribution in nickel-based superalloy under tensile loading up to 30% total strain.

Table 1. The material and its corresponding crystal structure

Figure	6(A)	6(B)	6(C)	6(D)	6(E)	6(F)
Material	RR1000 nickel-based superalloy	RR1000 nickel-based superalloy	26mm thickness pure titanium plate	Manufactured 316L stainless steel	RR1000 nickel-based superalloy	26mm thickness pure titanium plate
Crystal Structure	Face Center Cubic	Face Center Cubic	Hexagonal close-packed	Body Center Cubic	Face Center Cubic	Hexagonal close-packed

CPFEM simulation of a nickel-base superalloy nominated Haynes 282 was carried out, and the local elastic strain and plastic strain were collected and analysed through the Matlab application. Figure 7 shows the contour map of plastic strain after 2% total strain.

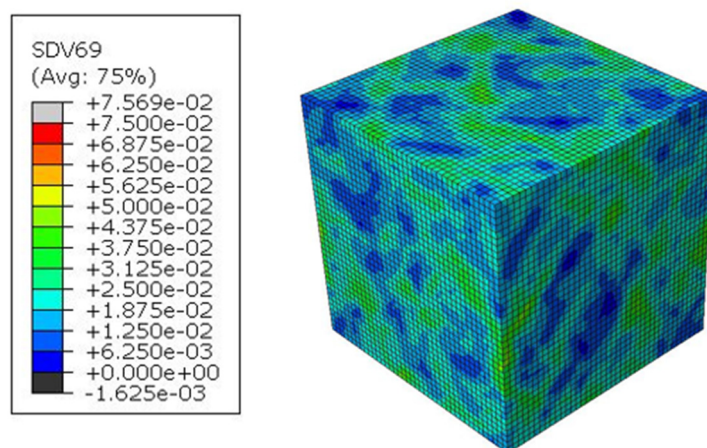


Figure 7. A contour map showing the plastic strain at 2% loading point

Figure 8-14 illustrate the distribution of local plastic strains and elastic strains between 2% and 30% loading stage, and all the data were well matched with the generalized extreme value fit. Considering the excellent fitting in Figure 6 (experiment data) and Figure 8-14 (simulation result), it is reasonable to assume that both local plastic and elastic strain follows generalized extreme value distribution regardless the crystal structure of the material and loading stage.

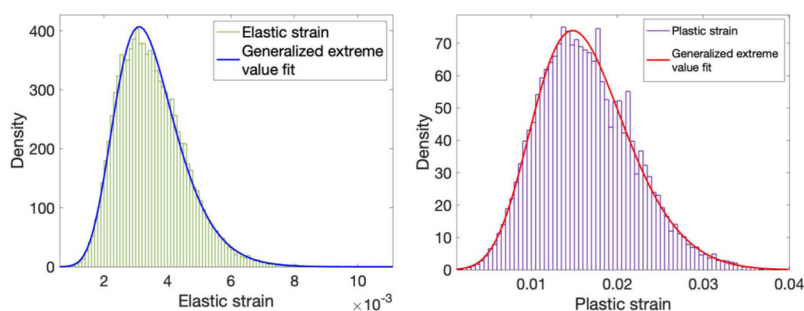


Figure 8. The distribution of local elastic strain and plastic strain when the total tensile strain reaches 2%.

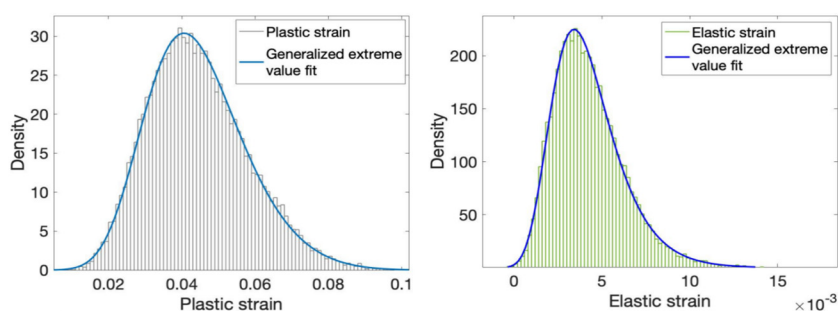


Figure 9. The distribution of local elastic strain and plastic strain when the total tensile strain reaches 5%

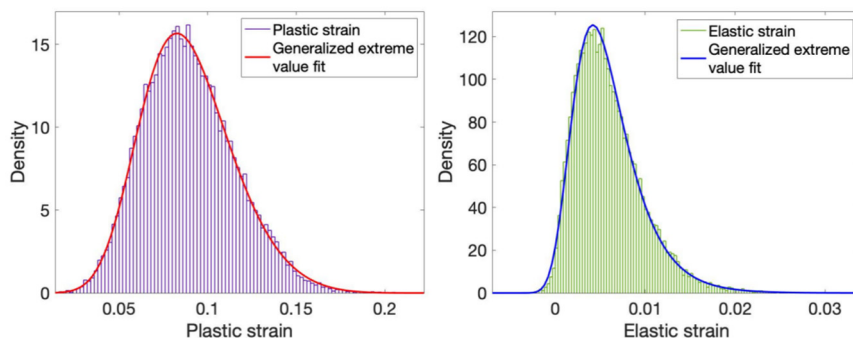


Figure 10. The distribution of local elastic strain and plastic strain when the total tensile strain reaches 10%

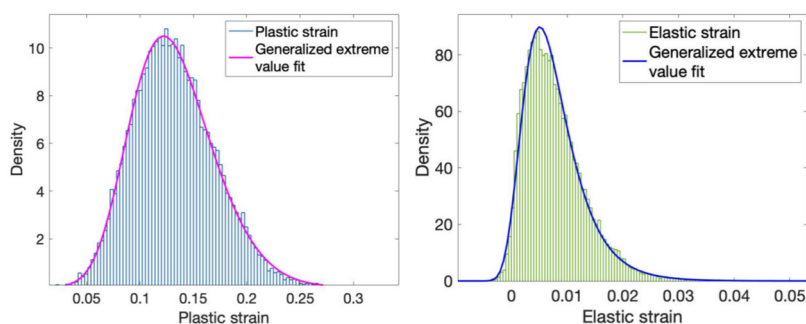


Figure 11. The distribution of local elastic strain and plastic strain when the total tensile strain reaches 15%

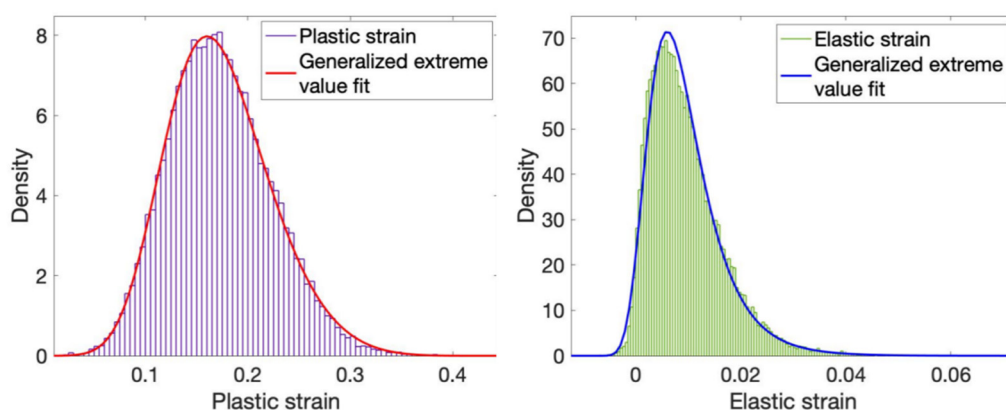


Figure 12. The distribution of local elastic strain and plastic strain when the total tensile strain reaches 20%

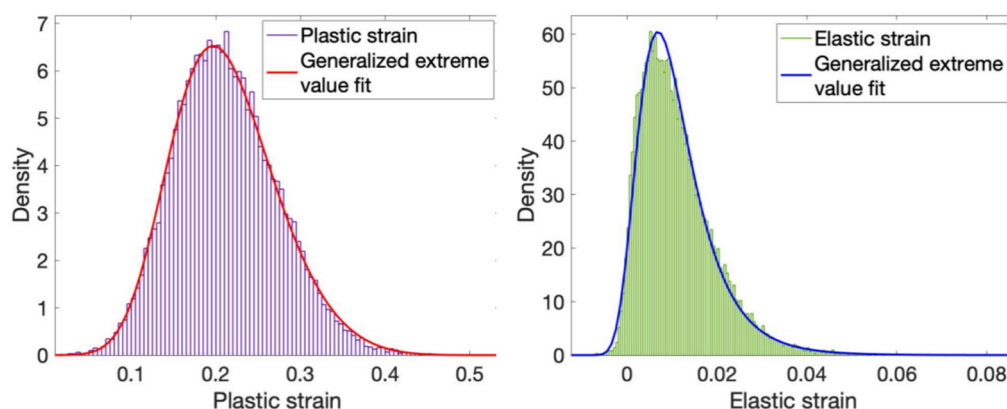


Figure 13. The distribution of local elastic strain and plastic strain when the total tensile strain reaches 25%

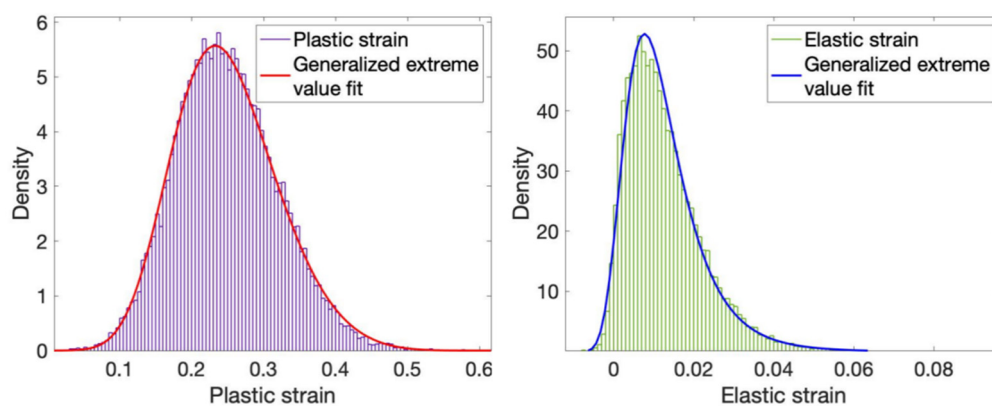


Figure 14. The distribution of local elastic strain and plastic strain when the total tensile strain reaches 30%

Table 2 lists all the generalized extreme value fitting parameters for Figure 8-14. It is apparent from Table 2 that the deviation of the distribution σ for both elastic and plastic strain increase when the total strain increases from 2% to 30%, which means that the local strain will have a boarder distribution as the total strain increases.

Table 2. The fitting parameter for Figure 8-14.

Loading stage	parameter	Parameter value	Parameter error
2% plastic strain	k	-0.136399	0.00395762
	sigma	0.00502362	2.39E-05
	mu	0.0140645	3.39E-05
2% elastic strain	k	-0.0740539	0.00398173
	sigma	0.00090621	4.37E-06
	mu	0.00303514	6.13E-06
5% plastic strain	k	-0.135753	0.00411376
	sigma	0.0122178	5.85E-05
	mu	0.0388264	8.28E-05
5% elastic strain	k	-0.0305286	0.00407644
	sigma	0.00163553	7.95E-06
	mu	0.0033641	1.11E-05
10% plastic strain	k	-0.150544	0.00325316
	sigma	0.0237486	0.00011043
	mu	0.0788437	0.00015782
10% elastic strain	k	0.00752032	0.00427405
	sigma	0.00293107	1.45E-05
	mu	0.00419744	1.99E-05
15% plastic strain	k	-0.150789	0.00271673
	sigma	0.0354785	0.000162868
	mu	0.116243	0.000233282
15% elastic strain	k	0.032023	0.00444057
	sigma	0.00409492	2.06E-05
	mu	0.00521254	2.80E-05
20% plastic strain	k	-0.155795	0.00246627
	sigma	0.0466926	0.000212839
	mu	0.152363	0.000305611
20% elastic strain	k	0.045008	0.00440245

	sigma	0.00514736	2.59E-05
	mu	0.00622458	3.51E-05
25% plastic strain	k	-0.160327	0.00230208
	sigma	0.0571211	0.000259049
	mu	0.186943	0.000372804
25% elastic strain	k	0.0574151	0.00462305
	sigma	0.00608921	3.11E-05
	mu	0.00718868	4.18E-05
30% plastic strain	k	-0.167185	0.00230203
	sigma	0.0670173	0.000303364
	mu	0.22068	0.000437307
30% elastic strain	k	0.0640715	0.0047138
	sigma	0.00697579	3.58E-05
	mu	0.0081317	4.80E-05

5. Discussion

Chen et al. studied the multiscale investigation of deformation heterogeneity in additively manufactured 316L stainless steel, and they emphasized that substructure colonies might be a new scale that plays a noteworthy role in local plastic strains and damage initiation [9]. Tang et al. reported the distribution of total strain follows a lognormal distribution. While Tang's research mainly focused on the total strain, they did not study the distribution of local elastic and plastic strains separately [1]. Additionally, Chen & Korsunsky investigated the statistics distribution of local stress and strain, and they separated the total strain into elastic strain and plastic strain. they discovered that elastic strain obeys normal distribution while strain conforms lognormal distribution. The small elastic strain (and stress) accumulation process is found to be additive leading to a normal distribution, whereas larger magnitude plastic strain can be well described by a lognormal distribution and obeys a multiplicative accumulation process [4]. However, in the current study, it is easily to find out that the strain (include total strain, elastic strain, and plastic strain) can well described by the generalized extreme value fit, which is different from the finding in the reference [1] and [4]. The advantage of generalized extreme value distribution over normal/lognormal distribution is that it can simultaneously describe all component of strain and total strain using only one type of distribution.

6. Conclusion

The aim of this work is to statistical distribution of plastic and elastic deformation in different type of polycrystalline materials. It is clear from the experiment data that the strain statistics obtained from all the materials with different crystal structure (HCP, FCC BCC) can be well described by the generalized extreme value fit. To further support the experimental finding, CPFEM simulation were carried out using the material property from a nickel-base superalloy nominated Haynes 282. All the strain distribution conforms to the generalized extreme value distribution. Therefore, according to the result obtained from the experiments and the simulations, It is emphasized that the distribution of

local elastic strain, plastic strain, and total strain can be well described by generalized extreme value for all type of polycrystalline materials under tensile deformation.

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