



Quantifying the severity of plastic strain localization in polycrystals

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ABSTRACT

Plastic strain localization is usually a precursor to ductile failure in polycrystals, with failure probability increasing as localization becomes more severe. However, the severity of localization is typically evaluated qualitatively or through imperfect quantitative approaches, limiting its practical relevance. In this article, we propose an analysis based on localization factors to quantify strain localization severity in polycrystals by drawing an analogy to the electric potential energy of clustered positive point charges. Specifically, we treat the spatial distribution of plastic strain as a system of point charges, where stronger aggregation indicates more severe localization. This method successfully quantifies localization in both synthetic strain distributions, experimentally measured strain distributions, and those in nanostructured Ag alloys from atomistic simulations, which exhibit enhanced strain localization when segregated with Cu at grain boundaries and reduced localization when segregated with Ni. More importantly, the approach combined with structural analysis can efficiently identify underlying localization mechanisms, including those not readily apparent in strain fields. By quantifying strain localization, this work demonstrates that strain fields contain far more information than previously recognized and introduces a versatile tool for identifying different deformation and failure stages and for analyzing material behavior across nano-, micro-, and macroscales, enhancing the ability to predict and understand material failure from a variety of strain maps.

1. Introduction

Plastic strain localization is a common and critical deformation mode of metallic materials under mechanical loading. During localization, plastic strain becomes heterogeneously distributed, with some regions experiencing intense deformation while other regions remaining largely unaffected. Depending on constitutive behaviors and loading conditions, strain localization manifests itself in various modes: necking in ductile metals under tension [1–6], shear banding in metallic glasses [7–12] or heavily cold-worked metals [13–20], Lüders banding in mild steels [21–26], persistent slip banding in metals under cyclic loading [27–33], and adiabatic shear banding in many materials loaded at very high strain rates [34–37].

Regardless of the modes, strain localization is usually associated with the failure of the deformed solids. On one hand, severe strain localization often precedes failure [38,39] as these highly deformed regions serve as preferential sites for crack nucleation. For example, in uniaxial tension, necking leads to void nucleation within the localized zone, ultimately resulting in fracture when these voids grow and coalesce [40].

A more extreme case is adiabatic shear banding, where numerous microvoids form and merge inside the band, causing abrupt failure [35, 41] even in the absence of cracks, as observed in the deformation of bulk metallic glasses [8,42]. In these cases, strain localization marks the transition from stable to unstable deformation process, making the localization severity a good indicator for material failure.

On the other hand, beyond these extreme cases where immediate failure happens right after strain localization, more localized strain concentrations, even without causing immediate failure, can also contribute to crack formation and promote material failure [43,44]. In crystalline materials, for instance, strain often localizes along slip planes during dislocation motion, forming persistent slip bands when dislocations repeatedly glide on adjacent atomic planes [38]. This localization can intensify when dislocations are blocked by grain or phase boundaries, resulting in steep strain gradients that promote crack nucleation and growth at dislocation-boundary intersections [45,46]. Persistent slip bands are also the primary precursors to fatigue failure in ductile metals under cyclic loading. The highly localized plastic deformation creates extrusions or intrusions on the sample surface [47–49], resulting

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in stress concentration and promoting crack nucleation. Conversely, crack formation itself can induce strain localization in brittle materials [50,51]. For example, under freeze-thaw cyclic loading, pores and micro-fissures can develop in localized regions of gneiss [52], reducing local shear strength, facilitating shear localization, and ultimately leading to failure.

Given the close relationship between strain localization and crack formation, it is crucial to evaluate the severity of localization to signify imminent material failure and to pinpoint the underlying failure mechanisms. This is typically accomplished by analyzing the spatial distribution of local strain, which can be obtained experimentally using digital image correlation (DIC) [53–55] or computed through various simulation methods such as finite element analysis [56,57], discrete element analysis [58], or atomistic simulations [59,60]. From these spatial strain distributions, localization severity is assessed by examining how and where the strain concentrates within the sample.

The most intuitive way to assess strain localization is to examine the spatial strain distribution map, which reveals when and where strong strain concentrations occur. The severity of localization can also be estimated from the intensity and spatial extent of these concentrated regions. Although this approach is widely used, it remains largely qualitative, even though the underlying strain fields are inherently quantitative.

Rice proposed a criterion to predict when and how localization may occur, but this quantitative framework does not assess the extent or severity of strain localization [61]. Also, past works used the coefficient of variation (CV), defined as the ratio between the standard deviation (SD) of distributed strain and average strain, as a metric to evaluate the localization severity [62–65]. Large CV usually means severe localization. Others used SD directly [66,67]. However, these approaches rely solely on statistical strain distributions. As a result, it cannot distinguish between cases where high strain is concentrated in a small region and cases where strain is uniformly distributed, if the overall statistical distributions are similar.

Analogous to the well-established stress concentration factor in mechanical engineering, the strain concentration factor, defined as the ratio between maximum local strain and nominal strain, has been used to quantify strain localization [68–70]. A large value indicates that the local strain is much higher than the average, suggesting strong localization. However, this metric remains limited because it does not distinguish between cases with different spatial strain distributions that should be regarded as having different localization severity.

Strain gradients have also been linked to localization severity [71–73], since large gradients indicate abrupt spatial variations in strain. However, this approach is typically applied only to highly localized regions, such as crack tips, necking front, or interfaces, and it neglects the role of strain magnitude in evaluating overall localization.

When deformation is dominated by shear banding, shear band width has also been used as a localization metric [74–76]. However, this measure is only applicable when a well-defined shear band forms and therefore cannot be generalized to more complex or diffuse localization modes.

Overall, the primary limitation of existing metrics is their insufficient treatment of the spatial pattern of strain distribution, which is the defining feature of strain localization. By definition, strain localization refers to the concentration of deformation within a specific region, yet this fundamental spatial characteristic is often not captured in quantitative analyses.

Spatial statistics seemingly offer promising tools for this purpose, for example Moran's I (a measure of spatial autocorrelation) [77] or Ripley's K function [78] (a measure of point-pattern clustering over distances). However, closer examination shows that these functions are not well suited to quantifying localization severity, despite explicitly incorporating positional information. Moran's I is bounded between -1 and 1 and indicates whether high or low values cluster in space, but it does not reflect strain magnitude. In contrast, strain localization has no

intrinsic upper bound, as its severity can increase with higher strain gradients or more concentrated deformation. Similarly, Ripley's K captures point density but treats all points equally, regardless of their strain values. Thus, although these metrics capture spatial arrangement, they lack the sensitivity to strain magnitude and gradients required to fully quantify localization severity.

In this article, we propose a novel strategy to quantify the severity of plastic strain localization by sufficiently incorporating both the magnitude and spatial arrangement of strain across a deformed sample. This strategy is inspired by the principle that multiple point charges of the same sign increase the total electric potential energy when they cluster together, and decrease it when they move apart. By analogy, we treat the strain at each position as a positive point charge and define *strain localization factors* (LFs) based on the total potential energy, providing a quantitative measure of strain localization severity.

LFs can assess strain localization in both synthetic strain distributions and in real strain distributions generated using DIC analysis or through atomistic simulations, with the LF values in agreement with expected localization behavior. In addition to quantifying the localization severity, the LF analysis can also aid in revealing the underlying strain localization mechanisms using nanocrystalline Ag-Cu and Ag-Ni alloys [60] as model systems. In the Ag-Cu alloys, homogeneous Cu segregation promotes strain localization, whereas in Ag-Ni alloys, heterogeneous Ni segregation tends to suppress it. By separately computing LFs in grain boundary (GB) and grain interior regions of each alloy, we reveal that homogeneous Cu segregation promotes not only localized GB sliding but also concentrated dislocation glide within grains. In contrast, heterogeneous Ni segregation suppresses GB sliding and leads to more uniform dislocation-mediated plasticity in the grain interiors.

These findings add new insight into the deformation mechanisms of these alloys and demonstrate the value of quantifying strain localization from another perspective. Overall, this work presents a versatile tool to extract critical information from spatial strain distributions, which can be used to gauge failure and gain deeper understanding of the deformation and failure mechanisms of materials.

The remainder of this paper is structured as follows. Section 2 describes the methodology, including the formulation of the LF metric, the construction of synthetic strain distributions, the DIC analysis of a 5050 Al alloy under uniaxial tension, and the atomistic simulations of Ag-Cu and Ag-Ni nanostructured alloys. Section 3 presents the LF results obtained from these three types of strain fields and compares them with other approaches introduced in Section 1. This section also discusses how LF analysis reveals the underlying mechanisms of strain localization. Section 4 summarizes the main conclusions and highlights the broader implications of this approach for quantifying strain localization severity.

2. Methodology

In this section, we first propose a formula for calculating the localization factor (LF) based on appropriate assumptions and considerations. We then generate various synthetic strain distributions to represent diverse localization patterns. Subsequently, we describe the preparation of experimental strain data obtained from digital image correlation (DIC). Finally, we present the details of the atomistic simulations performed on nanostructured Ag-Cu and Ag-Ni alloys.

2.1. Formulation of strain localization factor

The LF was computed by using the formula:

$$LF = \frac{1}{V} \sum_{i(j, \varepsilon_i) \bar{\varepsilon} > \bar{\varepsilon}} \frac{(\varepsilon_i / \bar{\varepsilon} - 1)(\varepsilon_j / \bar{\varepsilon} - 1)}{r_{ij}}, \quad (1)$$

where ε_i and ε_j are the strain at positions indexed with i and j , respectively, $\bar{\varepsilon}$ the average strain, r_{ij} the distance between positions i and j , and

V the sample volume. The factor is used to measure the intensity of strain localization, rather than the extent of strain. To ensure that the calculation was not affected by the latter, we normalized the strain at each position by the average strain over the sample volume. Because fracture typically occurs in highly strained regions, we only accounted for strain values higher than the average when performing the calculations. This formulation ensures that $\epsilon_i/\bar{\epsilon} - 1$ represents the positive point charge at position i , which is zero when the local strain equals the average strain and becomes negative when the local strain is below the average. As defined, the LF is zero for uniform strain distribution and is independent of V .

2.2. Preparation of synthetic strain distributions

To validate the proposed formula, we constructed a series of synthetic strain distributions in model samples. Each sample consisted of discrete points arranged in a simple cubic lattice with a lattice constant of 3 Å and periodic boundary conditions applied in all three directions. Beginning from a $75 \times 75 \times 150$ Å³ sample, artificial strain was imposed by assigning predefined strain values to selected points through nine different methods, as illustrated in Fig. 1.

In Figs. 1(a-c), a finite strain up to 0.5 was selectively applied to lattice layers while the remaining layers were assigned a zero strain. In Fig. 1(a), different strain magnitudes were assigned to the same middle layer to mimic shear bands of equal thickness but varying intensities. In Fig. 1(b), the number of adjacent layers with a fixed strain of 0.5 was changed to simulate shear bands of various thicknesses. In Fig. 1(c), five layers with a strain of 0.5 were distributed at different separations across the sample to evaluate the effect of spatial dispersion.

In contrast, the configurations shown in Fig. 1(d-f) were designed to

control and homogenize the average strain. In Fig. 1(d), the total strain was distributed across an increasing number of layers, while keeping the average strain constant, to diffuse the shear localization. As a result, the strain magnitude per layer decreases with increasing number of selected layers. In Fig. 1(e), selected layers were assigned a strain of 0.5, while the remaining layers were assigned varying strain values between 0 and 0.5. Fig. 1(f) extended this concept by also varying the strain on the selected layers to maintain a uniform average strain across the entire sample, ultimately producing a fully uniform strain distribution.

The final three cases shown in Figs. 1(g-i) explored the influence of sample dimensions on the LF computed in Eq. (1). In Fig. 1(g), the number of layers along the longitudinal direction was reduced while assigning a fixed strain of 0.5 to the middle layer, resulting in an increased average strain. In Fig. 1(h), a similar dimensional reduction was performed, but the strain value was adjusted to keep the average strain constant. In Fig. 1(i), the lateral sample dimensions were modified while maintaining a fixed strain of 0.5 in the middle layer, which did not affect the average strain.

2.3. Preparation of DIC strain data

A standard dog-bone uniaxial tensile specimen, with a thickness of 0.5 mm and a gauge dimension of 50 mm in the tensile direction and 8 mm in the lateral direction, was machined from 5050 Al alloy sheet for digital image correlation (DIC) strain measurement on an area of 47.6×6.4 mm² on the surface of the gauge section. Following surface preparation, a high-contrast random speckle pattern was applied to the gauge section to ensure optimal pattern quality for DIC correlation. The specimen was then mounted in a materials testing system and loaded under displacement control at a constant crosshead speed of 2 mm/min

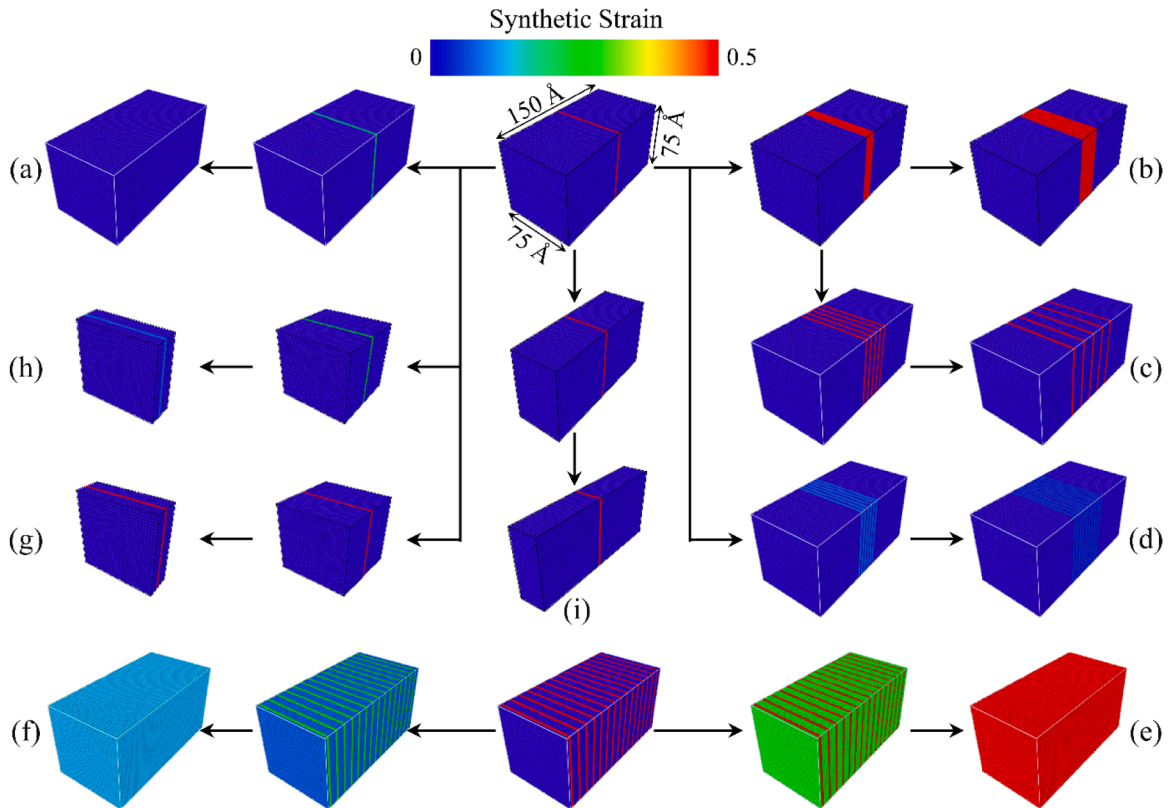


Fig. 1. Various spatial distributions of synthetic strain. The distributions were created based on an $150 \times 75 \times 75$ Å³ atomic configuration by (a) varying the strain value in the middle atomic layer, (b) increasing the number of neighboring layers with high strain, (c) creating different spatial distributions of strain with the same statistical distributions, (d) dispersing the strain to more layers while keeping the average strain a constant, (e) varying the strain values in low-strain regions, (f) distributing the total strain into more regions, adjusting the longitudinal sample size while (g) fixing the strain value in the middle layer or (h) keeping the average strain a constant, and (i) adjusting the lateral sample size while fixing the strain value in the middle layer.

and a corresponding strain rate of $2.5 \times 10^{-4} \text{ s}^{-1}$. Two industrial cameras with a resolution of 1280×1024 pixels were positioned normal to the specimen surface and synchronized to capture images at a rate of 1 frame per second throughout the entire test, from initial loading until final fracture. The acquired image sequences were processed using the DIC method described in a prior work [79], with a subset size of 31×31 pixels and a step size of 27 pixels. Finally, the DIC-derived strain fields were synchronized with the load-time records from the testing machine via trigger signals, producing full-field strain maps for subsequent strain localization analysis.

2.4. Atomistic simulations of Ag-Cu and Ag-Ni alloys

The Ag-Cu alloy and Ag-Ni alloy polycrystals were created by hybrid Monte Carlo (MC) and molecular dynamics (MD) simulations [80] in the software LAMMPS [81], using an embedded-atom method interatomic potential for Ag-Cu [82] and a Finnis-Sinclair interatomic potential for Ag-Ni [83]. Both systems were created based on a nanocrystalline nanotwinned Ag with an average grain size of 6 nm and twin boundary spacing of 2.8 nm that was constructed using Voronoi tessellation method in a $30 \times 30 \times 30 \text{ nm}^3$ cubic box with periodic boundary conditions applied in all three directions. The as-constructed model was first relaxed to its local minimum energy state with a conjugate-gradient algorithm and then equilibrated at 500 K under zero pressure for 50 ps. Thereafter, the model was doped every 100 MD steps with either Cu or Ni atoms of compositions up to 15 at. % by the MC method in a variance-constrained semi-grand canonical ensemble [80]. After equilibrium, the alloys were quenched from 500 K to 300 K for 100 ps and then kept at 300 K for another 100 ps at zero pressure with a Nose-Hoover thermostat [84] and a Parrinello-Rahman barostat [85]. Finally, uniaxial tension was performed in the X direction at a strain rate of 10^8 s^{-1} and a temperature of 300 K while maintaining zero pressure in other directions. After deformation, the strain tensor of each atom was calculated from the relative displacement of neighboring atoms. In other words, the deformation of each atom was calculated from the initial (reference) configuration formed by the neighboring atoms and the

deformed configuration formed by the same group of atoms [86,87]. Then the von Mises strain of each atom was calculated as input for the strain localization analysis. All visualization and structural analysis such as common neighbor analysis [88] other than the calculation of LF were performed using the open-source visualization tool OVITO [89].

3. Results and discussion

In this section, we first present the results of strain localization analysis using a series of carefully designed synthetic strain distributions. Next, we apply the analysis results based on experimental strain fields obtained from DIC measurement. We then employ localization analysis to examine strain distributions in nanostructured Ag-Cu and Ag-Ni alloys via atomistic simulations and elucidate the underlying localization mechanisms using the insights derived from LF calculations. Finally, we discuss the computational performance of the LF method and its sensitivity to various analytical parameters.

3.1. Strain localization factor in synthetic distributions

Fig. 2 presents the behavior of the LF for the various synthetic strain distributions introduced in Fig. 1. For comparison, the CV and SD of the imposed strain, which has previously been used in the literature to quantify strain localization [62–67], was also computed and included in the figure. Fig. 2(a) shows that LF remains constant despite the increasing strain value in the middle layer, while the SD increases proportionally. The constant LF output in this case arises from its normalization: the LF depends solely on the spatial distribution of nonzero strain and is mathematically equal to the reciprocal of the fraction of strained points, independent of the actual strain values. This indicates that LF is invariant with respect to changes in average strain and is thus insensitive to strain magnitude in this scenario. In contrast, the SD naturally incorporates both the spatial distribution and magnitude of strain and therefore increases as the strain intensity rises. This behavior implies that SD is more appropriate for quantifying the severity of strain localization in this case, whereas LF is not. However, it should be noted

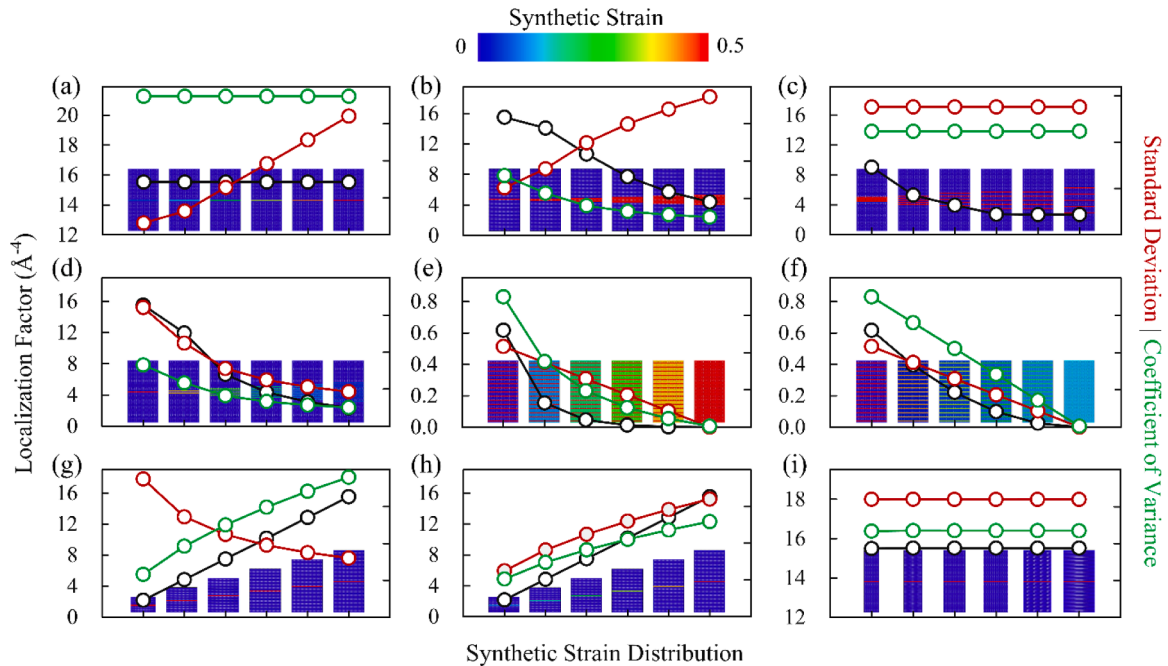


Fig. 2. The localization factor for all synthetic strain distributions. How the standard deviation and coefficient of variance change with various distributions (a-i) shown in Fig. 1 is also presented to make comparisons. The inconsistency in (b), (c), and (g) implies that standard deviation is not appropriate for assessing the severity of strain localization, while that in (c) shows that coefficient of variance is not appropriate either, making localization factor the most reliable metric to quantify the degree of strain localization.

that the SD is not normalized by the average strain. When the CV, i.e. the normalized SD is used, the same constant trend is observed. Therefore, while LF alone does not totally capture changes in strain magnitude, it can provide more meaningful information when considered together with the average strain, as shown in the following.

Fig. 2(b) illustrates the response of LF, SD, and CV when the number of adjacent layers with nonzero strain is increased. As the width of the localized strain region increases, LF exhibits opposite trend to SD, but same trend to CV: LF and CV decreases, whereas SD increases. This discrepancy again arises from the role of average strain in each calculation. In this case, the average strain increases with increasing localization width. While this effect is explicitly removed in the calculation of LF and CV, it is inherently included in the SD. Consequently, this case confirms that SD aggregates strain magnitude and spatial distribution, making it sensitive to the global strain level rather than just localization.

Although prior studies [90] have occasionally used the width of the high-strain region as a proxy for localization severity, Fig. 2(b) suggests that this approach conflicts with the precise definition of strain localization based on the LF. As high strain spreads across a larger portion of the sample, the deformation becomes more diffuse and therefore less localized, even if the average strain increases. Ultimately, if the entire sample experiences uniform high strain, no localization exists. This inverse relationship is correctly captured by the LF, which decreases with increasing strain spread, thereby aligning with the spatial confinement of deformation. In contrast, the SD increases, incorrectly suggesting stronger localization. These results underscore the importance of decoupling strain localization from average strain and highlight the advantage of LF as a more accurate and physically meaningful measure in such contexts.

Although Fig. 2(a-b) shows that CV follows the same trend as LF, the primary limitation of SD and CV as measures of strain localization is their reliance on the statistical distribution of strain values rather than on their spatial arrangement. In contrast, LF is explicitly defined from the spatial distribution of strain. This distinction becomes critical in cases where samples share identical statistical strain distributions but differ in spatial configuration. As shown in Fig. 2(c), such cases yield the same SD and CV values, whereas LF increases as the strain becomes more spatially localized. This demonstrates that SD and CV fails to distinguish between spatially distinct strain patterns when their statistical properties are equivalent. This scenario is uncommon but does exist in the deformation mode of materials, with single shear band and multiple shear band as typical examples.

Figs. 2(d-f) further illustrate cases in which LF, CV, and SD all align well with expected physical behavior. More diffuse strain distributions correspond to reduced localization, and the agreement arises from the similar statistical and spatial features of each synthetic distribution. However, this consistency breaks as the sample size changes. As shown in Fig. 2(g), LF and CV increase with increasing sample length, consistent with expectations because the strained region occupies a smaller fraction of the sample and deformation becomes more localized. In contrast, SD decreases with increasing sample size, reflecting its sensitivity to the decreasing average strain.

This discrepancy highlights the need to remove the influence of average strain by construction. When the average strain is held constant, LF, CV, and SD recover the same trend, as shown in Fig. 2(h), confirming that average strain is a major limitation in SD-based localization analysis.

Finally, Fig. 2(i) explores changes in the lateral dimensions of the sample while holding the longitudinal length and strain distribution fixed. In this case, LF, CV, and SD remain unchanged, which is consistent with expectations, as the strain distribution along the loading direction remains unaltered and lateral expansion does not influence localization in that direction.

In summary, SD fails to reliably measure strain localization because it reflects statistical distribution and is influenced by average strain, leading to misleading trends in cases like Figs. 2(b), (c), and (g). In

contrast, LF provides consistent and physically meaningful results by capturing spatial localization independent of average strain, as demonstrated in Figs. 2(d-f) and (h-i). Though CV provides meaningful results in most cases, it fails when the statistical distribution does not resemble the spatial distribution, as shown in Fig. 2(c).

In addition, other metrics can be used to quantify the localization severity, but all exhibit certain limitations. For instance, the strain gradient approach [71] would produce identical results for the distributions in Fig. 2(b) due to the identical boundaries between low- and high-strain regions. If the strain distributions in Fig. 2(c) corresponds to the same nominal strain, the strain concentration factor [68] would remain the same because the maximum strain values are equal. Moreover, Moran's I [77] would yield a value of 1 in Figs. 2(a), (b), (g), and (h), as high-strain regions all cluster together in these distributions. Likewise, Ripley's K function [78] would produce the same results in all of the inhomogeneous distributions in Figs. 2(e) and (f), since the spatial density of high-strain positions is consistent across these distributions regardless of the maximum and minimum strain values. Collectively, these limitations, alongside those of SD and CV, strongly suggest that the LF approach is the most robust metric currently available for quantifying strain localization.

It is important to note that materials can fail through different modes depending on sample geometry, constitutive behavior, and loading conditions. For example, metallic glasses under tension or compression fail rapidly through shear banding [8,9], making strain localization, as can be quantified by LF, a key indicator of impending failure. In contrast, ductile materials such as coarse-grained Cu undergo a prolonged stage of uniform deformation before necking and fracture occur. In such cases, failure may be accompanied with a relatively low LF value due to the low normalized strain values by the large average strain accumulated during the uniform plastic deformation process. In this case, the average strain has dominating effect on the failure and should be considered while using LF to assess failure. To explore this, we plotted LF versus average strain in Fig. 3 for all the synthetic strain distributions shown in Fig. 1. Except for cases with constant average strain, LF decreases as average strain increases. Since both high localization and large average strain contribute to failure, we define a new indicator, i.e., the *modified localization factor* (MLF), as the product of LF and average strain. As shown in Fig. 3, each MLF value defines an inverse relationship between LF and average strain, with higher MLF values indicating a higher likelihood of failure.

Fig. 4 shows how MLF varies across the different synthetic strain

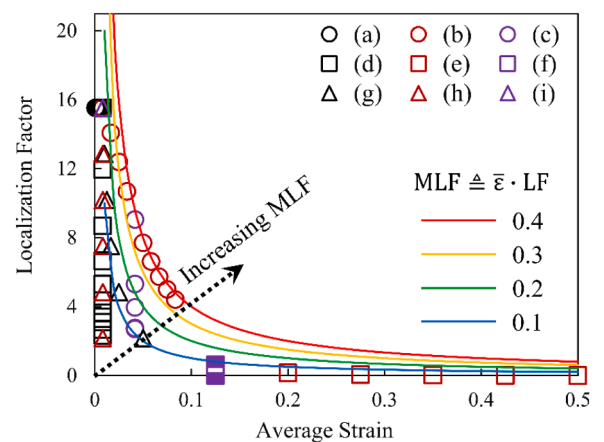


Fig. 3. The localization factor as a function of the average strain for various synthetic strain distributions. The data label follows the figure panel label in Fig. 1. Since both high localization factor and average strain promote failure, a modified localization factor defined as the product of the localization factor and average strain is proposed as another means to evaluate localization severity.

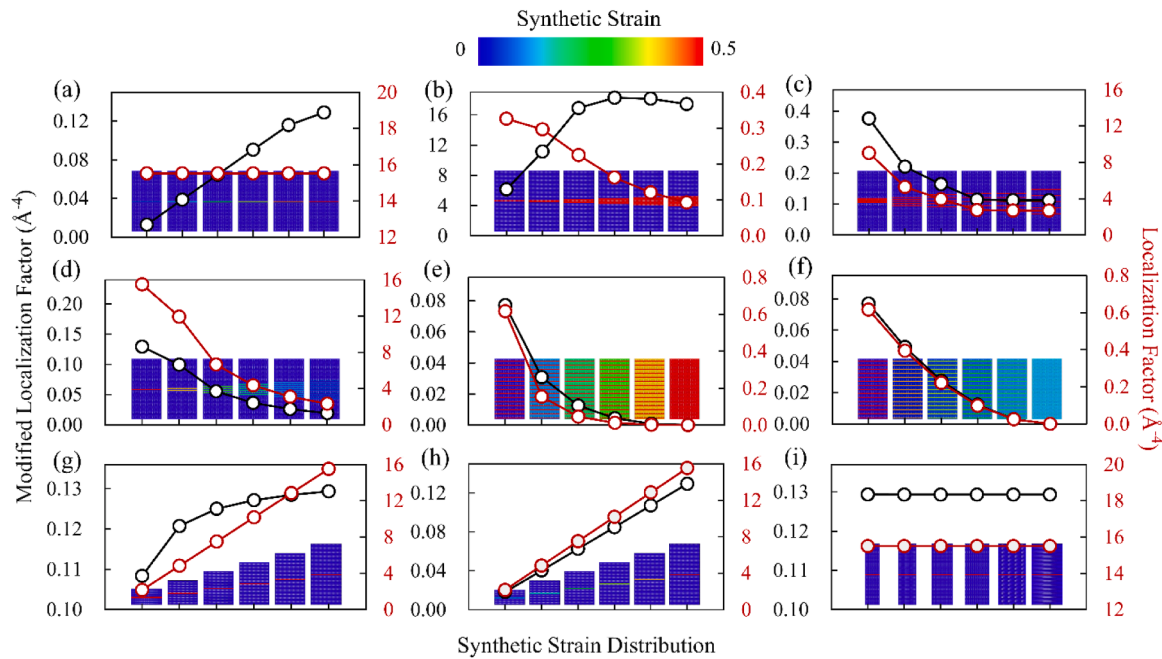


Fig. 4. Modified localization factor (MLF) for the various synthetic strain distributions. The localization factor of various distributions (a-i) shown in Fig. 1 is also presented to make comparisons. MLF shows some relative improvement in (a), (b), and (g) over predictions made from the localization factor in assessing the degree of strain localization.

distributions. Regardless of how the strain is distributed, the MLF trends are always consistent with physical intuition. For instance, Fig. 4(a) shows that MLF increases when higher strain is localized in the same region of the sample. MLF also aligns with the traditional view that more severe localization corresponds to a wider shear band. As shown in Fig. 4(b), MLF initially increases with band width, reaches a maximum, and then decreases as the band approaches the full length of the sample, eventually reaching zero when the strain becomes fully uniform. Additionally, MLF naturally captures size-independent localization behavior. As shown in Fig. 4(g), when strain localizes in the same region but the sample size varies, MLF converges to a constant value for sufficiently large samples. This further confirms that MLF is a more robust and physically meaningful measure of strain localization severity. The LF and MLF results across various strain distributions highlight a critical point: the effect of average strain must be removed from the LF calculations to ensure a general physical consistency. While this removal might occasionally yield LF values that appear counterintuitive for some specific cases, the average strain can always be added back to modify the calculation results to ensure consistency in all cases. Therefore, LF and average strain should be treated as independent variables that can be recombined when necessary.

It should be noted that the introduction of MLF serves as one illustrative example of how LF and average strain can be combined to create a metric for quantifying strain localization. How MLF is defined is also simply based on the physical intuition that failure probability should increase when either LF or average strain increases. While this form is a straightforward way to naturally capture this synergistic effect, failure depends on a variety of factors and are often much more complex. For materials that deform via Lüders banding [21] severe strain localization occurs early, yet the failure LF might be small. Consequently, MLF might decrease during the deformation, as shown in Fig. 4(b) and (c), if we treat the synthetic strain maps as a sequence of a deformation process. The MLF at failure could also be lower than at the initial deformation stage, rendering it ineffective as a failure indicator. In such cases, MLF, if used as a failure indicator, should be redefined (e.g., as the product of LF and the square of the average strain) to increase the weight of average strain. Therefore, MLF in the current form should not be regarded as a

universal indicator for failure. Other combinations of LF and average strain may be necessary, and additional factors may need to be incorporated to establish a more robust predictive criterion from strain distribution maps. Ultimately, new metrics based on LF can always be defined to assess the likelihood of failure according to the specific constitutive behavior of the materials of interest.

3.2. Strain localization factor in DIC strain distribution

Fig. 5 illustrates the evolution of the LF in a 5050 Al alloy during uniaxial tension, based on the strain distribution data obtained from DIC analysis [79]. Fig. 5(a) displays the superimposed DIC images at critical stages, which is defined according to the LF curve presented in Fig. 5(b). Shortly after tension begins, at a tensile strain of only 0.00002, the LF rapidly rises to its highest value across the entire deformation process. The corresponding DIC image reveals that while strain across the sample is generally very low, one localized region exhibits a relatively higher strain concentration, even though its absolute value remains small. This relatively high-strain region later extends to a larger area, indicating that yielding likely initiates from this location.

The pronounced early peak in LF arises from normalizing local strain values by an extremely low average strain at the onset of deformation. This sensitivity indicates that LF calculations can be unstable during the initial stages of deformation. However, provided that the strain distribution is accurate, the LF peak is indicative of the true onset of yielding. In ductile materials, yielding marks the initiation of plastic deformation well before final failure. Therefore, LF may serve not only as an indicator of imminent failure but also as a metric for detecting yielding.

This high LF value drops rapidly to a very low level once the applied tensile strain increases to 0.002. As shown in Fig. 5(a), both the local and average strain levels rise at this stage, reducing the normalized strain values and thus the LF. At a tensile strain of 0.005, the LF rises again to a high value. The corresponding DIC image shows that yielding has propagated into wider areas. Subsequently, the LF decreases markedly and remains low for an extended period, reflecting uniform deformation across the sample, as confirmed by the DIC images at tensile strains of 0.1 and 0.2.

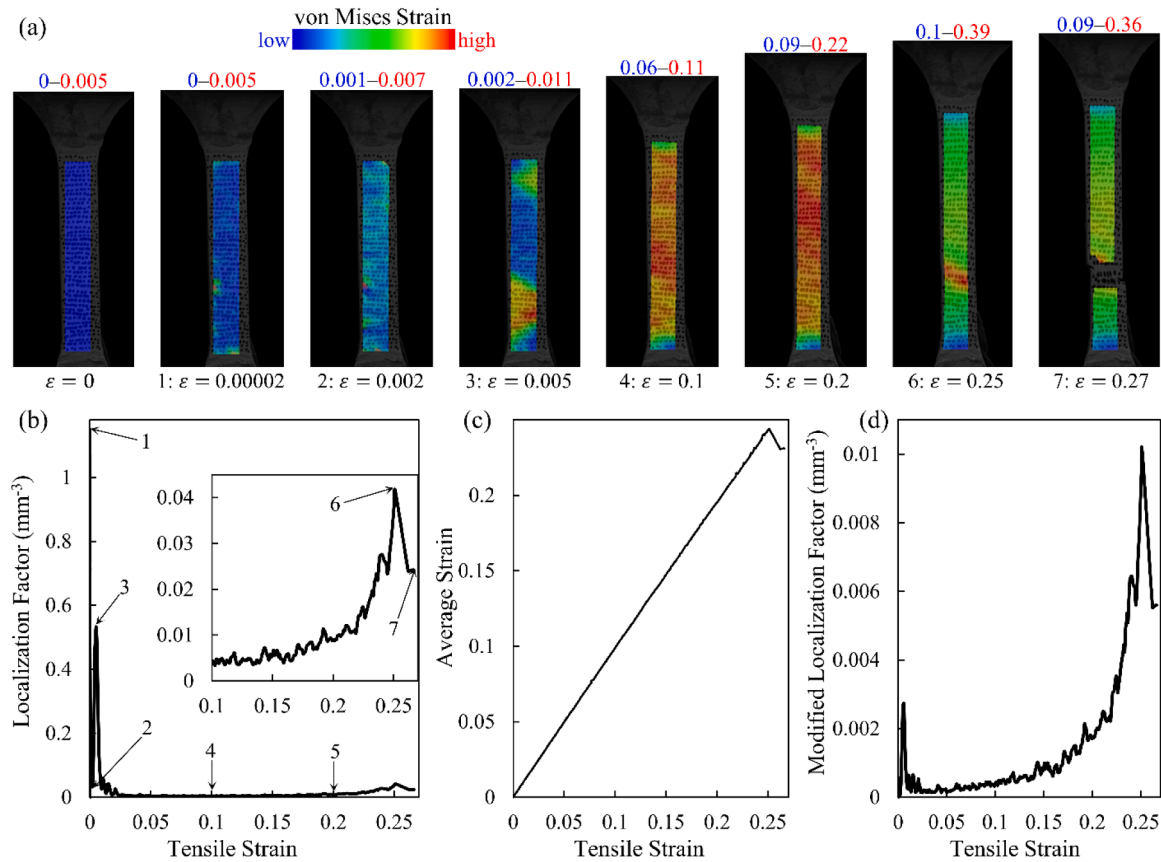


Fig. 5. Strain localization analysis based on experimentally measured strain distributions using digital image correlation (DIC). (a) Superimposed DIC images showing von Mises strain distributions on the 5050 Al alloy sample surface during uniaxial tension at deformation stages defined in (b) the localization factor (LF)-tensile strain curve. The strain range of the scale bar is varied to best show strain variance across the sample surface. The inset to (b) is a close-up of this curve at tensile strains from 0.1 to 0.27, showing that the LF increases quickly with increasing applied tensile strain before failure. (c) The average von Mises strain increases linearly with applied tensile strain until failure occurs. (d) The modified localization factor as a function of the applied tensile strain.

At a tensile strain of 0.25, the LF reaches another peak. The corresponding DIC image shows strain localizing again into a single region, followed rapidly by failure at a strain of 0.27. This stage represents severe strain localization immediately preceding fracture. Throughout deformation, the average strain accumulates nearly linearly with the applied tensile strain until reaching a peak value at applied strain of 0.25, as shown in Fig. 5(c). This indicates that the sample undergoes a prolonged stage of uniform deformation, requiring substantial average strain accumulation before failure occurs.

We also calculated the MLF at each applied strain. Fig. 5(d) shows that MLF also exhibits a noticeable jump at the onset of deformation, influenced by the initial LF spike. However, due to the very low average strain, this jump remains modest in magnitude. The MLF quickly declines and then increases gradually until a tensile strain of about 0.15, after which it rises more sharply until peaking at the onset of failure. This behavior indicates that MLF can serve as a criterion for material failure in this case. While average strain could also be used, its nearly linear evolution provides limited information about the deformation stage. In contrast, the MLF curve captures the progression of localization, including yielding and final failure, making it a more informative indicator of plastic deformation.

Though motivated by the connection between strain localization and failure, the LF analysis on DIC strain maps shows that high LF values, i.e. severe localization, does not necessarily mean failure. This implies that LF cannot be used as a failure indicator unless only failure is responsible for the localization. As a quantitative tool, however, LF itself does not distinguish between different physical events but only shows when and where localization occurs. Determining whether a high LF corresponds

to yielding, uniform deformation, shear banding, or pre-failure instability requires additional context and analysis.

Fig. 5 only shows a typical uniform plastic deformation mode. Some other materials, for example, 5XXX series Al-Mg alloy system, might deform through Luders [91] and/or PLC banding [92]. The common feature is that strain localizes into propagating or repetitive bands during deformation, yet the sample continues to deform stably, as evidenced by ongoing strain hardening (albeit serrated in the case of PLC). This intermittent stable-unstable cycle is particularly instructive because it challenges the intuitive notion that pronounced strain localization necessarily signals imminent failure.

Applying our LF method to these phenomena yields insights that align with the mechanical behavior revealed by the stress-strain curve. Consider two scenarios that commonly occur in such deformation modes: (1) individual bands broaden as deformation progresses, and (2) multiple bands nucleate and propagate across the sample. Intuitively, broader bands or a higher density of bands may suggest increasingly severe localization. However, as shown schematically in Figs. 2(b) and 2(c), our LF calculation reveals the opposite trend: the degree of strain localization decreases as bands widen or multiply. This decrease in LF corresponds precisely to the stabilization reflected in the ongoing strain hardening of the stress-strain curve. In other words, LF correctly captures the stable feature of such deformation modes despite the seemingly unstable appearance of the strain map.

This consistency again demonstrates that LF provides a physically meaningful measure of localization severity and could potentially distinguish between benign localization (e.g., propagating Luders or PLC bands accompanied by hardening) and critical localization that precedes

failure (e.g., the sharp LF increase before fracture in Fig. 5b) by tracking LF throughout the deformation process.

The versatility of LF and MLF extends beyond their original goal as indicators of material failure, suggesting broader applicability to problems involving spatial strain distributions. Because material failure is commonly analyzed within the framework of fracture mechanics, LF and MLF could potentially be further developed to estimate key fracture parameters, such as stored energy and fracture driving force, including the stress intensity factor K or J -integral. In fracture mechanics, stored energy accumulates until it reaches a critical level that triggers crack propagation. It is therefore reasonable to hypothesize that the evolving strain field around a crack tip, particularly as propagation is approached, contains information related to these fracture parameters. By analyzing such strain fields using LF, it may be possible to establish a quantitative relationship between LF-based metrics and conventional fracture mechanics measures. For example, a strong correlation between LF and K or J would imply that higher LF values correspond to higher fracture driving forces. If such relationships are confirmed in future studies, LF-based indicators could provide a means of estimating K and J directly from strain maps, offering a practical and experimentally accessible complement to traditional fracture mechanics analyses.

3.3. Strain localization factor in nanostructured Ag alloys

Finally, we used LF and MLF to analyze the deformation of nanostructured Ag alloys based on strain distributions generated through atomistic simulations. Our prior work revealed that homogeneous Cu segregation in nanocrystalline nanotwinned Ag promotes strain localization, whereas heterogeneous Ni segregation suppresses it [60]. As shown in Fig. 6, Cu segregates uniformly at GBs, while Ni forms heterogeneous, localized clusters. This difference in segregation behavior directly influences their deformation mechanisms. In Ag-Cu alloys, the homogeneous distribution of Cu facilitates strain localization during tensile deformation. Fig. 7 illustrates how increasing Cu concentration (from 0 at. % to 15 at. %) shifts the deformation mode from uniform to localized strain distribution. In contrast, the heterogeneous clustering of Ni in Ag-Ni alloys effectively hinders strain localization, as evidenced by the absence of shear bands even at higher Ni concentrations (Fig. 8).

The contrasting deformation behaviors of these two alloy systems serve as an ideal test case to validate our computational methods for analyzing strain localization in atomistic simulations. While we have proposed two mechanisms to explain these behaviors, GB thickening and enhanced GB sliding in Ag-Cu alloys versus Ni-rich clusters impeding slip in Ag-Ni alloys [60], these conclusions were initially qualitative assessments. However, some key insights may have been overlooked in such analyses. Our quantitative evaluation approach aims to clarify these points by uncovering finer mechanistic details and providing a more comprehensive understanding of strain localization

and uniform deformation in these systems.

Based on the von Mises shear strain distribution depicted in Figs. 7 and 8, we calculated the LF for both alloys and pure nanostructured Ag during tensile deformation. Fig. 9(a) reveals that the LF of pure Ag increases rapidly at the initial stage of deformation but soon stabilizes to a constant value as plastic deformation progresses, indicating that pure Ag deforms in a relatively uniform manner. In contrast, the LFs of both alloys remain relatively unchanged at the early stages of deformation until a strain of ~ 0.04 , with an abrupt increase in the LFs thereafter. However, beyond a tensile strain of ~ 0.06 , the LFs of the two systems diverge significantly. For the Ag-Cu alloys, the LF continues to rise with increasing tensile strain, exhibiting higher values for higher Cu concentrations. In contrast, the LF of Ag-Ni alloys quickly plateaus, regardless of Ni concentration. These trends are consistent with the observation in Figs. 7 and 8: the increasing LF of Ag-Cu alloys accurately reflects the strain localization behavior, and the saturated LF of Ag-Ni alloys underscores the suppressing effect of heterogeneous segregation on strain localization.

We also calculated the average shear strain during deformation. Despite the distinct deformation behaviors, Fig. 9(b) demonstrates that both alloys, irrespective of solute concentration, exhibit similar average shear strain across the samples. However, these values are consistently lower than those of pure Ag at the same tensile strain. This suggests that homogeneous and heterogeneous segregation have a similar effect on the overall average shear strain despite their distinct effect on strain localization, highlighting the complex role of solute segregation in governing deformation mechanisms.

Considering that polycrystalline materials deform through a combination of GB-mediated and dislocation slip activities, we separately calculated the LFs for GBs and grain interiors based on the atomic shear strain in these regions. Fig. 9(c) reveals that the LF at GBs in Ag-Cu alloys is consistently higher than that in Ag-Ni alloys, indicating that GB plasticity is more localized in Cu-segregated Ag. This finding is consistent with our prior work [60] showing that homogeneous segregation of Cu promotes GB sliding by increasing the GB thickness, while heterogeneous segregation of Ni blocks GB sliding.

Another intriguing aspect is that the LFs of the grain interior in both alloy systems also exhibit notable differences. Fig. 9(e) shows that the LF of the grain interior in Ag-Cu alloys is also significantly higher than that in Ag-Ni alloys. This effect suggests that strain localization in Ag-Cu alloys is not solely attributed to localized GB plasticity but also arises from dislocation slip events that are more localized in Ag-Cu alloys. To test this hypothesis, we revisited the atomic configurations of deformed Ag-Cu and Ag-Ni alloys with a solute composition of 15 at. % at a tensile strain of 0.1 in Fig. 10. It is evident that Ag-Cu deforms primarily through strain localization along GBs, whereas localized GB sliding is blocked in Ag-Ni. However, close inspection reveals that the shear band in the Ag-Cu alloy does not exclusively follow GBs but also cuts through

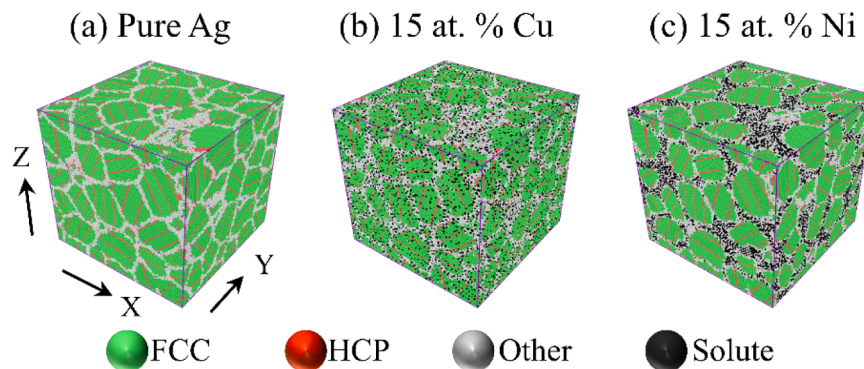


Fig. 6. The equilibrium configuration of nanostructured metals used in atomistic simulations. (a) Pure Ag, (b) Ag alloy with homogeneous Cu segregation, and (c) Ag alloy with heterogeneous Ni segregation. The face-centered cubic (FCC), hexagonal densest packed (HCP), and other permutations of atoms are colored green, red, and white, respectively, and solute atoms (Cu or Ni) are highlighted in black.

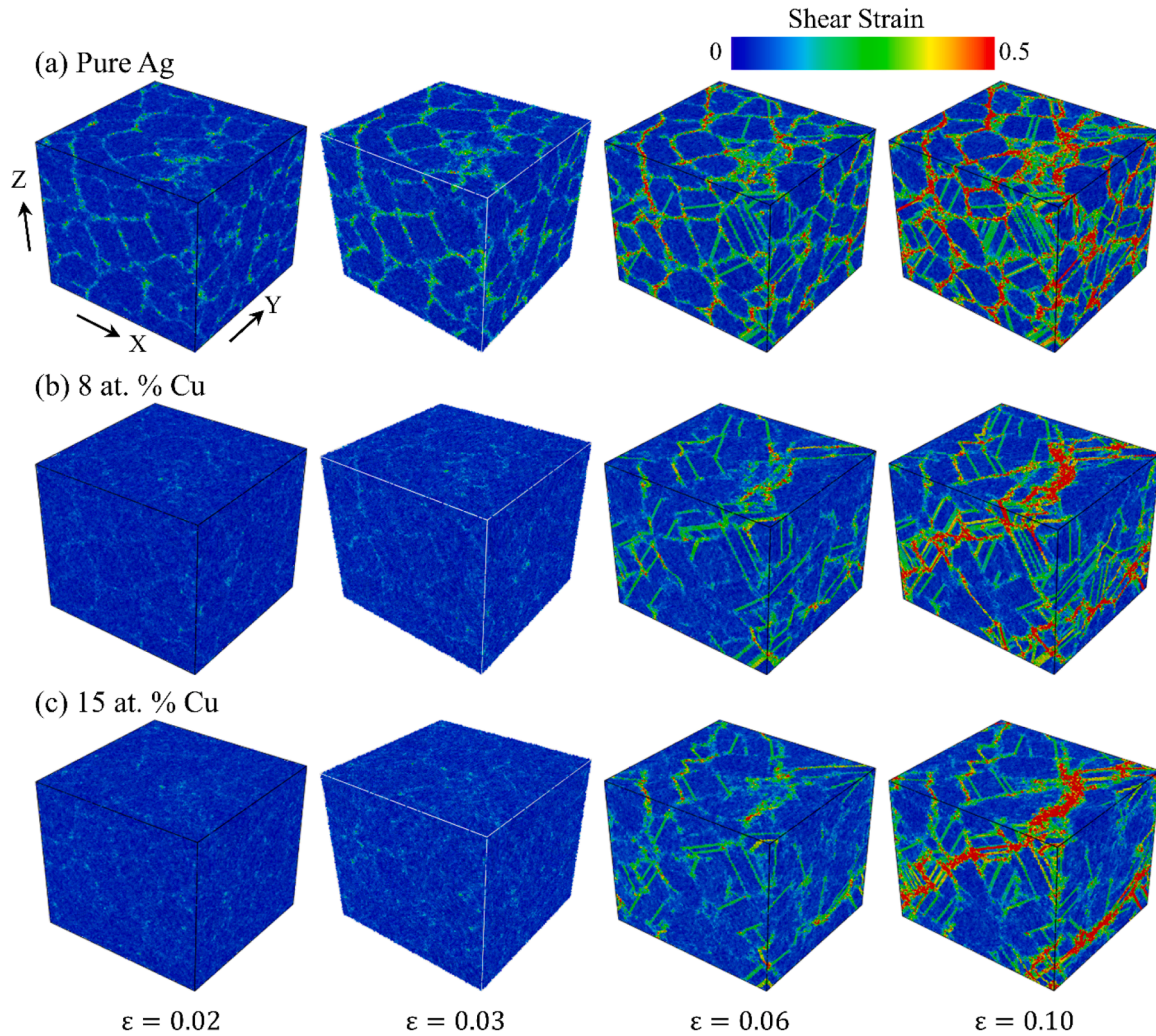


Fig. 7. Atomic von Mises shear strain distributions inside Ag and Ag-Cu alloys. (a) Pure Ag, and Cu-segregated Ag alloy at (b) 8 at. % Cu and (c) 15 at. % Cu, demonstrate strong strain localization in Cu-segregated nanocrystalline Ag, which is absent in pure Ag.

certain grains, with the straight high-strain bands bridging two GBs indicating dislocation slip bands, as shown in the marked regions in Fig. 10(a). In other words, strain localization does not only involve localized GB sliding but also induces concentrated dislocation slip along the localized regions, resulting in high LF within the grain interior of Ag-Cu alloys.

In contrast, Ni-rich clusters formed during heterogeneous segregation effectively block both GB sliding and dislocation slip in Ag-Ni alloys. While GB sliding is confined to GBs and is entirely suppressed when blocked, dislocations within grains have multiple slip directions. When some dislocations are obstructed by the Ni-rich clusters, new dislocations can nucleate and propagate along alternative directions. Consequently, dislocations in Ag-Ni alloys move in various directions, leading to extensive yet uniform plastic deformation within the grain interiors. This behavior is reflected in the lower LF and more homogeneous strain distribution observed in Ag-Ni. These findings highlight the merit of LF in quantifying the severity of strain localization.

The value of calculating the LF is further illustrated by analyzing the strain localization of pure Ag during tensile deformation. Although significant GB sliding is observed in the early stages of deformation, the LF at GBs remains relatively low, indicating that GB sliding occurs in a rather uniform manner, as shown in Fig. 9(c). Therefore, the initial rise in the overall LF should be attributed to the high LF within the grain interior. As shown in Fig. 9(e), the LF of the grain interior in pure Ag increases rapidly after a tensile strain of 0.01. This suggests the possible

occurrence of dislocation slips, even though snapshots of the atomic configurations do not provide direct visual evidence. To verify this hypothesis, we conducted a dislocation analysis on the sample and indeed identified the presence of partial dislocations within a few grains. These dislocations, embedded deep within the sample, were easily overlooked because the entire sample appeared to show no dislocation movement at this stage. This result underscores the ability of the LF-based approach to reveal subtle deformation mechanisms that could be overlooked otherwise.

When combined with average strain analysis, this approach yields additional insights. Fig. 9(d) shows that the average shear strain at GBs in Ag-Cu alloys is consistently higher than that in Ag-Ni alloys, with the difference diminishing with decreasing solute concentration. In addition, the average shear strain at GBs in both alloys is significantly lower than that of pure Ag, consistent with the usual understanding that solute segregation suppresses GB sliding. However, the grain interior shows a contrasting behavior. As shown in Fig. 9(f), the average shear strain within the grain interior of Ag-Cu alloys is consistently lower than that of Ag-Ni alloys and pure Ag. This indicates that homogeneous segregation of Cu localizes and suppresses not only GB sliding but also dislocation slips, as evidenced in Fig. 10(a). In contrast, heterogeneous segregation of Ni does the opposite, as evidenced by the average shear strain levels close to those of pure Ag in the grain interior (Fig. 9(f)). These results elucidate the distinct roles of Cu and Ni segregation in governing deformation mechanisms, both at GBs and within grain

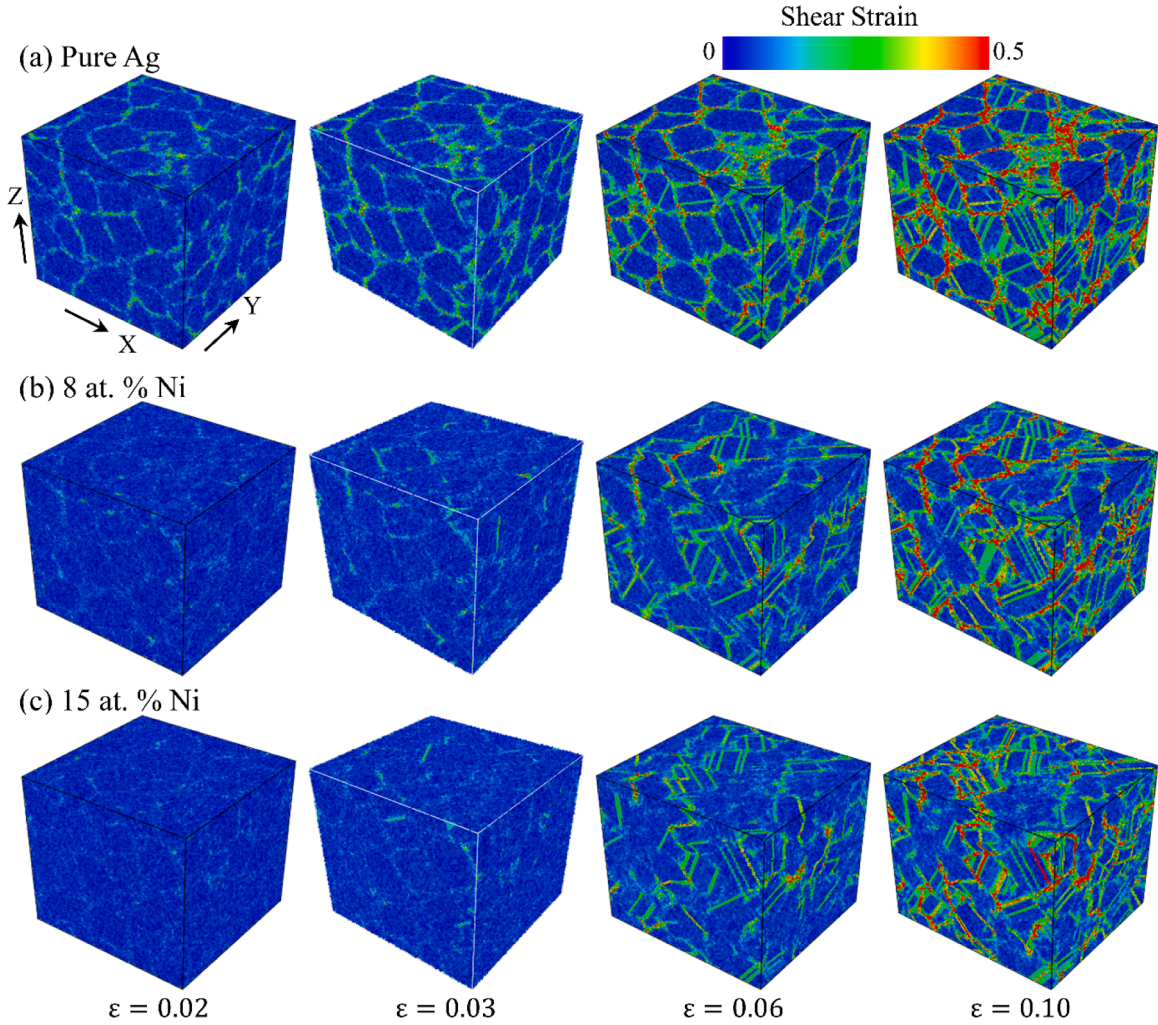


Fig. 8. Atomic von Mises shear strain distribution inside Ag and Ag-Ni alloys. (a) Pure Ag, Ni-segregated Ag alloy at (b) 8 at. % Ni, and (c) 15 at. % Ni, demonstrate no strong strain localization during the deformation process.

interiors, offering new insights into their influence on material behavior.

We also plotted the MLF as a function of tensile strain in Fig. 11. The LF against the average shear strain was plotted as well to provide more information. Figs. 11(a-b) show a strong localization trend in Ag-Cu alloys and uniform deformation in pure Ag and Ag-Ni alloys, consistent with Figs. 8(a-b). Figs. 11(c-d) confirm that strain localization in Ag-Cu alloys is predominantly driven by GB sliding. For the grain interior, Fig. 11(e) shows that LF of Ag-Cu alloys increases quickly with average shear strain, suggesting a strong strain localization resulted from localized dislocation activities along the shear bands (Fig. 10(a)). However, due to the large average strain, the MLF of pure Ag in the grain interior is higher than both alloys, as shown in Fig. 11(f). This MLF-based analysis reveals that strain localization in the pure nanostructured Ag metal is predominantly controlled by intragranular slip localization rather than GB-mediated plasticity, contrary to the deformation mechanisms in Ag-Cu and Ag-Ni alloys, where both dislocation and GB plasticity play important roles.

Although LF itself does not distinguish between different physical mechanisms, its application to nanostructured Ag alloys, particularly when combined with complementary structural analysis, demonstrates that LF can effectively uncover underlying localization mechanisms, especially those not readily apparent in strain fields. By quantifying strain localization through LF, this work demonstrates that strain fields contain far more information than previously recognized. Therefore, integrating LF with structural analysis offers a powerful means to

identify deformation and failure mechanisms, whether or not they are accessible through conventional analysis.

3.4. Computational performance and sensitivity analysis

The LF calculation involves computing pairwise distances for all points in a strain map, an operation that scales with $O(N^2)$, where N is the number of points. While acceptable for systems containing a few thousand points or less, this scaling is not for large-scale atomistic simulations dealing with millions or even billions of atoms. Fortunately, the electrical potential energy decreases rapidly with increasing separation distance between point charges. Beyond a certain distance, the contribution becomes negligible. This allows the introduction of a cutoff distance, limiting the search to point pairs within this range, a strategy commonly employed in atomistic simulations while calculating atomic interactions. By implementing an optimized neighbor search along with space-indexed storage methods, such as organizing point coordinates into array bins with bin size defined by the cutoff distance and the index reflecting their spatial relationships, the calculation of pairwise distances can be roughly limited between neighboring points defined by the cutoff. Since the number of neighbors of each point is usually far less than the total number N , the time complexity can be reduced to $O(N)$ approximately. This technique has been widely used in large-scale atomistic simulations. As a result, the LF calculation can handle a number of points comparable to the number of atoms in such

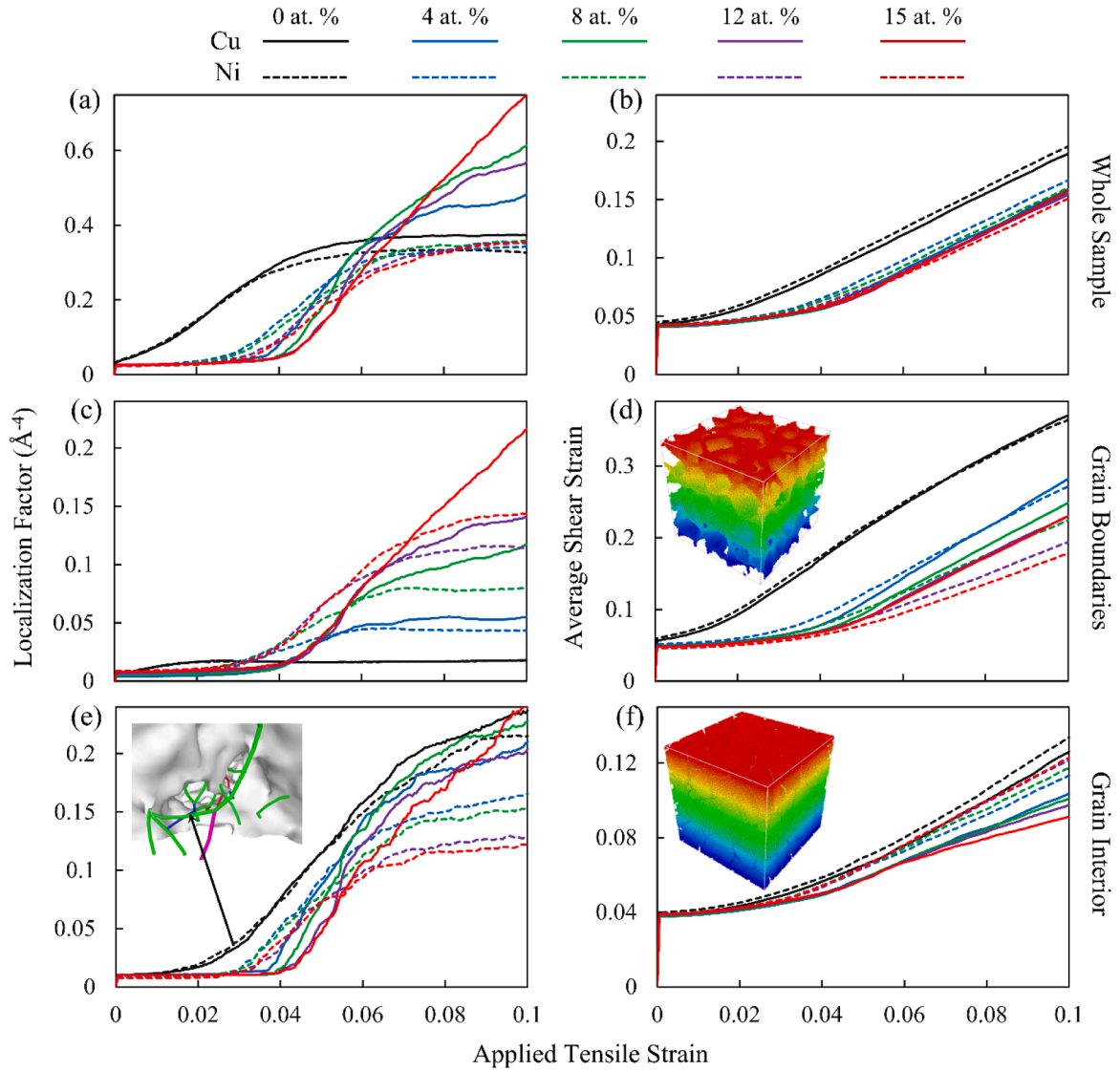


Fig. 9. Localization factor and average shear strain as a function of applied tensile strain. The results in (a, b) whole samples, (c, d) GB network, and (e, f) grain interior, respectively, indicate that the degree of localization of Cu-segregated Ag alloy is almost always higher than that of Ni-segregated Ag alloy, despite the close average strain. The inset to (e) shows the partial dislocations inside some grains of pure Ag at the early deformation stage. The insets to (d) and (f) show the atomic configurations of the GB network and grain interior, respectively.

simulations.

This raises the question of how to choose an appropriate cutoff distance. A large cutoff captures most significant contributions from points with high strain values, but at a high computational cost. Conversely, a small cutoff speeds up calculations but risks underestimating interactions from point pairs beyond the cutoff distance, leading to inaccurate results. A balance is therefore necessary.

As a practical guideline, the cutoff should be able to span a few heavily localized strain regions visible on strain distribution maps to include the contribution of large-strain regions to the total LF. These areas might cluster together or disperse in the map with an average separation distance. A small cutoff might fail to distinguish distributions with relatively large separation distances. For instance, in Fig. 2(c), the last few strain distributions might be given identical LF values if the cutoff is too small. However, as long as the cutoff is larger than the separation distance in the most dispersed cases, the requirement will be satisfied in all cases. In practice, a reasonable cutoff can be easily estimated by reviewing the available strain maps and approximating the maximum separation distance between localized strain regions in the most diffused distribution.

The computational cost can also be adjusted by varying the threshold strain, which is the value above which points are considered "high strain" and contribute to the LF. In our calculations, this threshold was set to be the average strain, based on the empirical observation that failure typically initiates in high-strain regions. Though having captured the essential features of strain localization across all cases presented in this work, this value can be adapted to specific material behavior not studied here. If failure occurs at a strain higher than the average, the threshold can be raised accordingly. This reduces the number of qualifying points and thus lowers computational cost. Conversely, if failure initiates at a strain below the average, the threshold can be lowered to include more points, which increases both the computational cost and the resulting LF value. Therefore, the choice of threshold is case-dependent. Nevertheless, based on our understanding and experience, the average strain generally serves as an appropriate and practical threshold, consistent with its use as the reference value in the calculations of CV.

It is worth noting that the strain threshold should always be relative to the average strain, because the average strain increases with the deformation process. If an absolute strain threshold was used, most

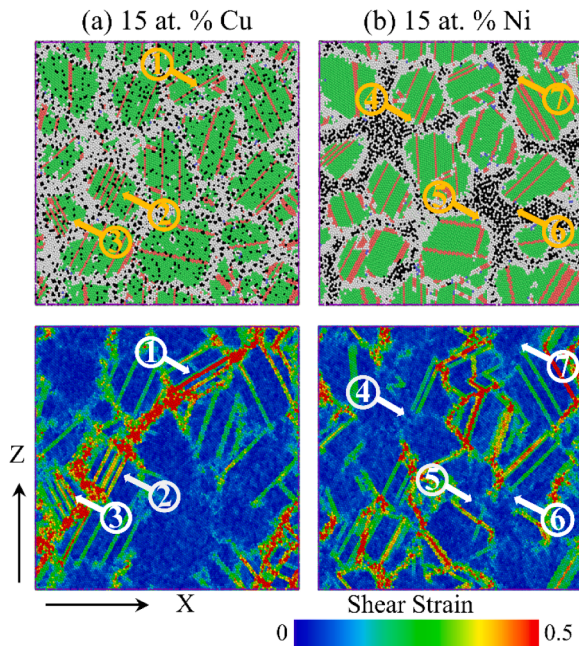


Fig. 10. Detailed close-up images illustrate the mechanism of plastic deformation when subjected to a 10% tensile strain and 15 at. % solute concentration. (a) Cu-segregated nanocrystalline Ag. (b) Ni-segregated nanocrystalline Ag. The solute atoms are visually represented in black, while local shear strain is shown underneath. The analysis reveals that strain localization triggers the dislocation movement within areas marked as 1, 2, and 3 in (a), whereas the dislocation movement is impeded by areas marked as 4, 5, 6, and 7 in (b).

strain points would fall below the threshold at early deformation stages and be excluded in LF calculation but exceed the threshold at later stages and be included in the calculation, introducing a deformation-biased inconsistency that distorts the interpretation of LF evolution.

LF is calculated from the positions of points, corresponding to pixels in DIC strain maps, making it inherently sensitive to image resolution that is affected by subset size and step size. For identical physical strain distributions, a higher-resolution image contains more pixel points per unit area, reduces the relative distance between neighboring points, and consequently increases the calculated LF. Conversely, a lower-resolution image will significantly reduce LF. Taking an extreme case as an example, when a high-strain region is represented by only a single pixel, its contribution to the total LF would likely be negligible. Therefore, to ensure a valid and meaningful LF analysis, the resolution of the strain map must be sufficiently high to accurately resolve the underlying strain features. In addition, when making comparisons, LFs must be calculated based on the images with the same resolution. Comparison between strain maps of different resolutions requires adjusting the resolution of these images to the greatest common divisor of the resolutions of these images and averaging the strain values of neighboring $n \times n$ points into a single point, with n being the quotient of the image resolution divided by the common divisor.

Although normalized by total volume, LF can still be sensitive to sample size, depending on whether the change in size affects the physical nature of the strain localization. As shown in Fig. 2(g), when the sample size is increased along the direction that change strain distribution profile, the strain appears more localized relative to the increased size, which raises the LF value. In contrast, Fig. 2(i) illustrates a scenario where the change in sample size does not alter the fundamental pattern of strain localization, and therefore LF remains unchanged. Therefore, if comparison has to be made between samples of different sizes, the size should not affect LF significantly, requiring that the sample should be large enough to remove the size effect on the deformation behavior and

the resulted strain map.

For polycrystalline metals, grain size also influences LF. If plastic strain initiates at GBs, as evidenced by the pure Ag in Fig. 7, larger grains tend to result in a higher calculated LF because the GBs are more widely spaced, concentrating strain in fewer, more distinct regions. In contrast, smaller grains, with their higher density of GBs, can lead to a more diffuse strain distribution and lower LF. This creates a challenge when directly comparing LF values between different grain sizes, especially in atomistic simulations, as a higher LF does not necessarily indicate a more severe or dangerous form of localization in a material failure context. However, this is not a limitation of the LF calculation itself. The issue lies in establishing a valid comparative metric for localization severity across different microstructures.

Nevertheless, when DIC is used to measure strain distributions, the resulting strain field has a low spatial resolution compared to that obtained from atomistic simulations. For instance, in our experiment, the subset size for DIC analysis is approximately $1.3 \times 1.3 \text{ mm}^2$, whereas the average grain size in coarse-grained metals is typically tens of micrometers. Consequently, the strain measured for each subset represents the average over an area containing roughly 2000 grains. This averaging effectively eliminates the influence of individual grain size variations. As a result, direct comparisons between different grain sizes become feasible, provided that the strain field resolutions and measurement dimensions are consistent across these samples.

Finally, it is important to consider the influence of noise in DIC strain maps. Noise can skew strain values across the map and affect LF calculations. If the noise level is nontrivial, particularly when it approaches or exceeds the average strain, it can artificially increase LF by introducing falsely high strain values. This is usually problematic in the early stages of deformation when actual strains are low. The largest error brought by the noise can be estimated from the first deformed strain map during deformation. However, as deformation progresses and true strains surpass the noise level, the impact of noise on LF diminishes. At this stage, noise primarily increases the average strain value used for normalization, which has a lesser, often negligible, effect provided that the noise level remains well below the true average strain.

4. Conclusions

In this work, we have proposed an efficient approach to quantify the severity of plastic strain localization based on how the electrical potential energy of multiple point charges changes with charge distributions. By treating large relative strains as point charges and defining LF as the corresponding potential energy, we have successfully analyzed strain localization in various synthetic strain distributions, those experimentally measured using DIC analysis, and atomic-scale strain distributions. Based on the results shown here, the following conclusions can be drawn.

- (1) Localization analysis based on well-chosen synthetic strain distributions shows that LF and MLF consistently quantify localization severity in agreement with expected physical behavior. In contrast, other proposed metrics, such as SD, CV, and Moran's I do not simultaneously account for strain magnitude and spatial information, and therefore fails in specific cases. This makes the proposed LF and MLF framework a more robust and physically meaningful measure of strain localization.
- (2) Localization analysis using experimental strain distributions from DIC confirms that both LF and MLF reliably quantify the severity of localization. Moreover, these factors effectively captured both the yielding stage and the final failure stage, further validating the robustness of the proposed quantification approach.
- (3) Our approach also aids in identifying underlying deformation mechanisms in atomistic simulations. By comparing the contrasting plastic deformation behavior of nanostructured Ag, Ag-Cu, and Ag-Ni polycrystals, we uncovered mechanistic insights

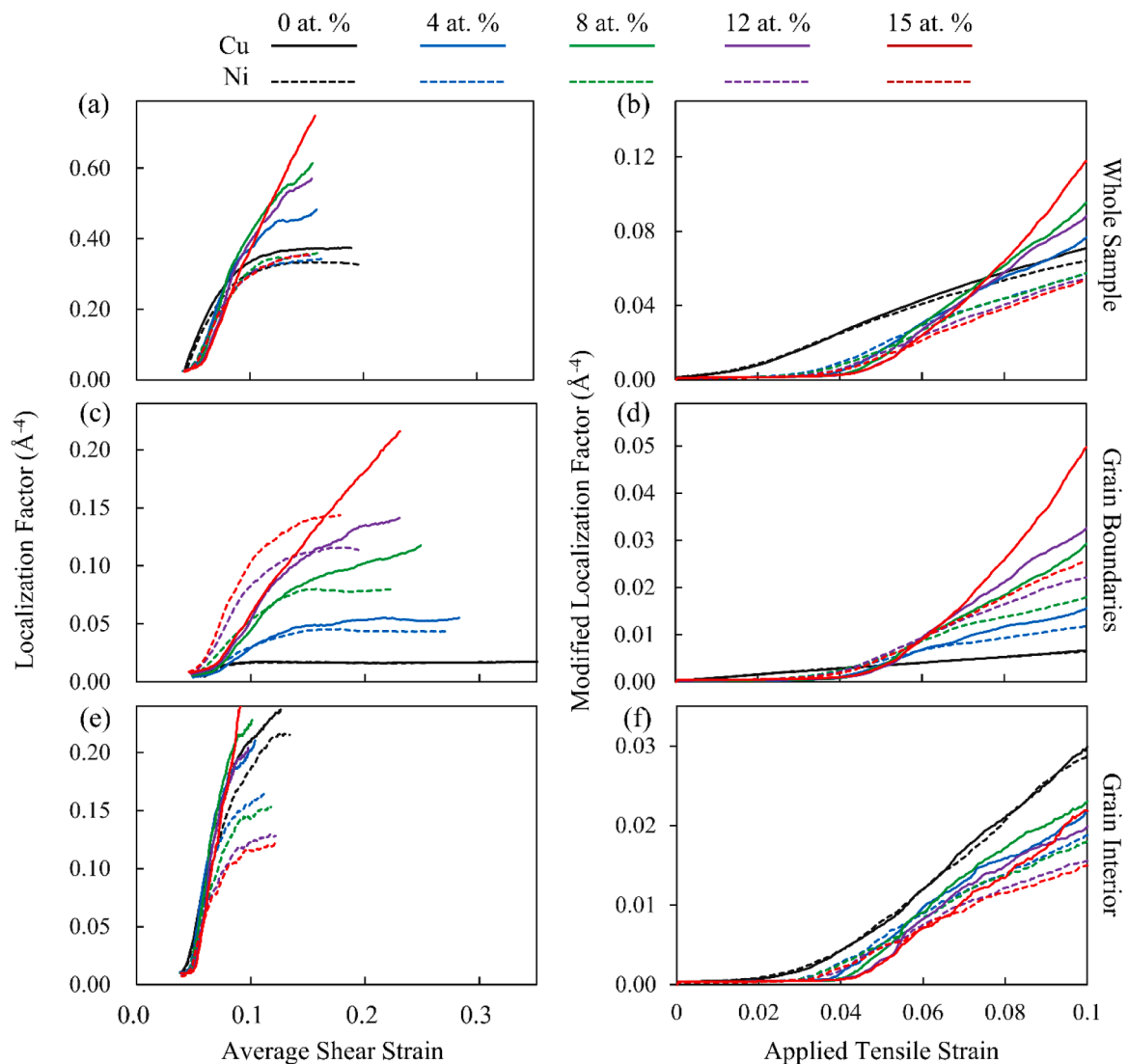


Fig. 11. Localization factor against average shear strain and modified localization factor versus applied tensile strain. Factors for (a, b) whole samples, (c, d) grain boundaries, and (e, f) grain interior, give the same information as shown in Fig. 8 about the degree of strain localization.

into strain localization that would be inaccessible without this method. Specifically, we found that homogeneous Cu segregation not only promotes localized GB sliding but also induces localized dislocation slip along the same regions. In contrast, heterogeneous Ni segregation suppresses both localized GB sliding and dislocation slip, resulting in a more uniform strain distribution within grains.

The results presented here show that our approach is broadly applicable. Whenever spatial strain distributions are available, whether from simulations or experiments, this method can quantify the severity of strain localization and identify its underlying causes by combining with structural analyses across different sample regions. Thus, this study introduces a versatile tool for identifying different deformation and failure stages and for analyzing material behavior across nano-, micro-, and macroscales, enhancing the ability to predict and understand material failure from a variety of strain maps.

CRediT authorship contribution statement

Peng Duan: Writing – original draft, Visualization, Software, Methodology, Investigation. **Frederic Sansoz:** Writing – review &

editing, Validation, Supervision, Funding acquisition, Formal analysis, Data curation. **Zhiliang Pan:** Writing – review & editing, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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