HIGH STRENGTH AND DUCTILITY ACROSS SIZE SCALES: 3D PRINTED METAL MATERIALS WITH MICROSCALE HETEROSTRUCTURE

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Abstract: Additive manufacturing (AM), also known as 3D printing, has made it possible for aeronautical structures to bear large loads while maintaining a low weight. However, due to the microscale heterogeneity caused by the AM process, almost all metal materials produced through AM exhibit different mechanical properties from conventional cast or wrought materials. In this study, the author applied numerical simulations based on a modified strain gradient theory to investigate the strength-ductility relationships of metal materials with heterostructures. The simulation results were in good agreement with experimental and literature data. A mechanism-based theory combining both statistically stored dislocations and geometrically necessary dislocations was used to depict the mechanical response across size scales. The study revealed that the Taylor stress and back stress dominate the high mechanical performance of materials with heterogeneous structures. Moreover, the width of the hetero-zone boundary affected region (HBar), which seems to be a constant dependent on the materials of the two phases, was found to be the key factor influencing the microscale heterogeneous materials. The results showed that metals with heterostructures possess superior mechanical properties exceeding the prediction by the rule-of-mixtures. Understanding the detailed influence of HBar may help enhance the strength of structures built using AM techniques with the same materials. These findings shed light on the mechanisms of the strength-ductility of materials with heterostructures across size scales and promote the design and manufacture of aeronautical AM structures to a higher level.

Keywords: Additive manufacture; Heterostructure; Size effect; Strain gradient theory

INTRODUCTION

In the aeronautical and aerospace industry, weight reduction has always been a goal pursued by scientists and engineers. In addition to traditional weight reduction methods such as hollowing and perforation, new optimization techniques such as topology optimization have also brought more convenient means for lightweight structural design, enabling structures to better conform to their load paths. For some components such as aerospace engine turbine blades, intricate internal structures are required for better heat dissipation to control blade temperature. Nevertheless, traditional manufacturing processes such as casting and cutting require huge time and material costs for the production of these parts, and some cannot even be manufactured. In contrast, additive manufacturing (AM) technology with its unique "discrete-stack" forming method has become a powerful tool for producing lightweight and complex structures. At present, there are various AM techniques available (such as laser/electron beam/arc AM methods, and powder/wire materials) that differ in terms of difficulty, efficiency, cost, advantages and disadvantages. However, the inherent metal melting-casting process of melting-pool-cooling-forming-stacking is fundamentally similar. This means that the melting-solidification behaviour of metals has a significant impact on the final properties of AM materials, making it one of the important research topics for AM methods today.

Many aeronautical and aerospace companies and suppliers are utilizing AM to produce lighter and stronger structural components, such as the tail fin fixator structure used for Airbus A350WXB shown in Figure 1(a) and the RUAG satellite antenna bracket shown in Figure 1(b) [1]. These load-bearing structures have been well optimized and can carry larger structural loads with a lighter weight. AM can significantly reduce the assembly quantity for the structure shown in Figure 1(a) and improve the fatigue damage tolerance of the structure, while the structure shown in Figure 1(b) is almost impossible to produce using traditional methods and can only be achieved through AM to realize such optimization. Figures 1(c)-(e) respectively show the MGT6100 gas turbine static blade, Siemens SGT-400 turbine blade, and GE company LEAP engine fuel nozzle [2]. These turbine engine hot-end components usually have precise shape designs, and AM can greatly improve the efficiency of traditional manufacturing and corresponding assembly steps. In addition to aeronautical and aerospace components, AM is also used in other fields, such as the 3D printed dental crown shown in Figure 1(f) [3], as well as other applications such as repair and life extension shown in Figures 1(g) and (h) [4]. Despite the remaining challenges in the principles, technologies, and techniques of AM, it still gradually plays a greater role in many fields due to its advantages in material efficiency and time efficiency over traditional manufacturing.

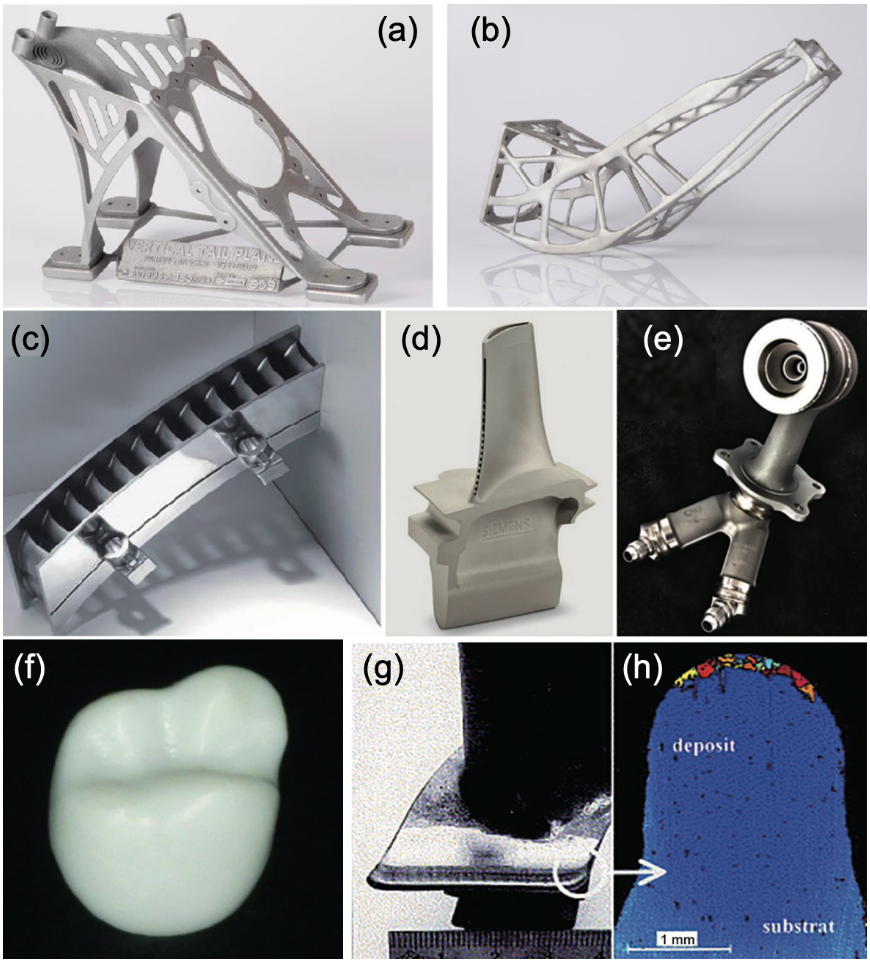

Figure 1: Examples of advanced additive manufacturing in different fields [1-4].

In order to use AM methods and products more efficiently, stably, and safely in the future, researchers have conducted many research works on various aspects of AM methods. Currently, scientists and engineers are primarily focused on the crystal microstructures (metals), printing precision improvement, and printing size extension. However, the "discrete-stacking" manufacturing process of AM, especially with the current printing precision reaching the micron level, can bring significant size effects to the products. This means that all material properties are closely related to their characteristic length. For example, for crystalline materials like metals, the smaller the grain size, the higher the material strength, stiffness and hardness. Fleck et al. found that the torsional stiffness of fine copper wires is related to their diameter, with a 12 μm diameter wire having a torsional stiffness about three times greater than a 170 μm wire [5]. Not only that, but scholars have also found that the microstructure of materials is closely related to their macroscopic properties, particularly for materials with heterogeneous structures. For example, shells have a typical micro-brick wall structure, exhibiting markedly different mechanical properties in the thickness and length directions of the bricks [6]. Due to the characteristic length of both hard inorganic and soft organic substances in the brick wall structure being in the micron scale, significant size effects are also observed. Ultimately, this design enables the shell to achieve a high load-bearing capacity with a lightweight and small structure. Also, it is worth mentioning that the growth of these shells is a generalized and sophisticated bi-material AM. Upon these findings, many cross-scale constitutive theories were suggested to better describe materials with a microscale characteristic length, the theory used in present work is also based on one of the cross-scale constitutive theory which is suitable for crystal materials and especially metals and alloys [7,8].

The metal materials produced by AM are always highly non-uniform. This heterogeneity comes from many aspects. First, the parts produced by AM typically have a certain structural design with designed heterostructures (if it is to produce bulk materials, AM has almost no advantages over traditional manufacturing methods). Second, AM has significant anisotropy in the layering and perpendicular directions. This anisotropy is an important characteristic of AM. Although it cannot be completely avoided, it can be minimized by designing the material to be printed at different angles, with load-bearing stress mainly designed to be in the printing plane rather than in the stacking direction [9]. Third, the manufacturing process of AM is similar to a series of "micro-welding", where new metal powders are melted and solidified together with the previously printed material. As the melting pool moves, non-uniformities related to its shape and path are gradually printed. Fourth, the repeated melting and solidification of metals, as well as different temperature (bottom/middle layer of printing, central/edge regions) can cause crystals to grow in different environments, resulting in microscopic heterogeneity [10]. Fifth, there are designed heterogeneities introduced, such as the printing of multiphase materials [11]. Such heterostructures usually provide some improvements to material performance, and the reason inside this phenomenon is the main purpose of this work.

The heterogeneities of interest in this paper mainly belong to the fourth and fifth categories mentioned above, one of which is difficult to avoid but its negative impact can be minimized through mechanical analysis, appropriately utilizing these heterostructures may even improve the mechanical properties of the material. In addition, the non-uniform characteristics unique to AM can be leveraged by intentionally designing microstructures to enhance the material's mechanical performance. However, referring to existing literature, it is found that the microscale heterostructures resulting from AM generally reduce the material's performance, such as fatigue and fracture, and there are relatively few reports of improvement in material properties.

HETEROSTRUCTURE AND MECHANICAL PROPERTY

The microstructure of AM materials has been studied by many researchers. This "micro" ranges from millimeter to micrometer. In millimeter scale, for example, Carroll et al. built an AM Ti–6Al–4V cruciform component and studied the tensile property of different positions and directions, as shown in Figure 2 [9]. The result showed that different samples have a similar elastic behavior, while in plastic deformation part, all AM materials' ultimate stress are about 5-10% higher than the wrought baseplate but the ultimate strain are much smaller than the wrought baseplate, especially the longitudinal sample. Although the characteristic length of the macroscale heterostructure involved here is on the order of millimeters, the materials produced by AM still exhibit certain high-strength, low-ductility properties. This also somehow confirms that although the overall performance of materials produced by AM is not yet comparable to that of traditional manufacturing, there are still unique advantages that, if better designed and utilized, will undoubtedly exceed the comprehensive mechanical properties of traditional materials.

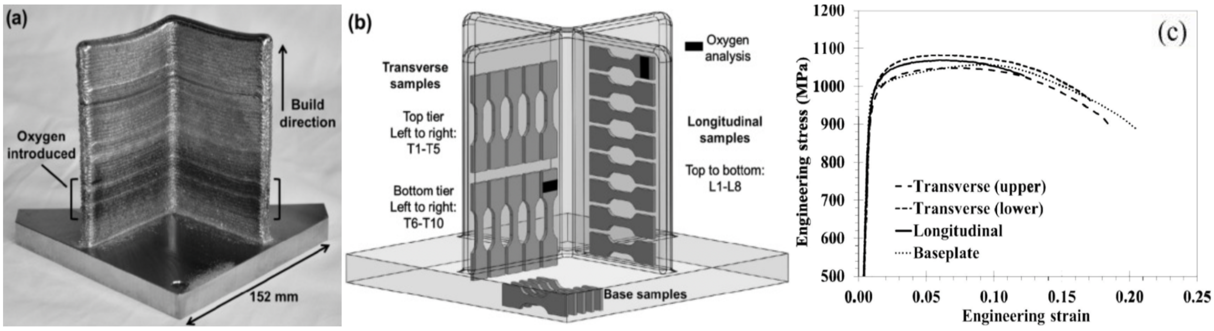

Figure 2: DED fabricated Ti-6Al-4V component and tensile tests from samples of different position and directions.

At the microscale, mechanical property is significantly influenced by micro-heterogeneity. AM method involves complex crystal growth behavior, with the main features being the crystal grain shape, orientation, and size at the grain scale (Figure 3 (a), [12]), as well as the ratio of the coarse and fine grains, interface density and distribution, impurities, porosity, and clusters at the domain scale (Figure 3 (b), [9]).

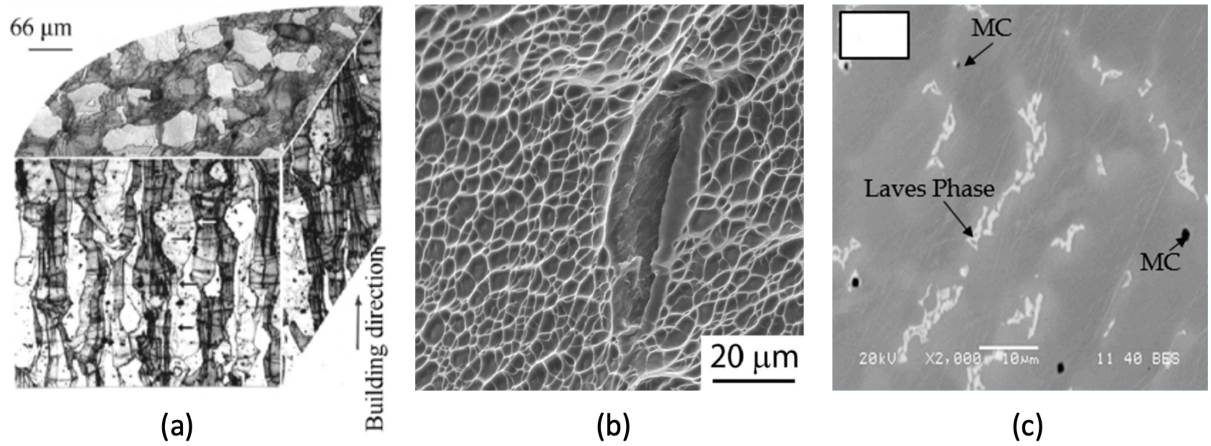

Figure 3: The microscale heterostructures and heterogeneities of AM metal materials.

These microstructures exhibit material size effects. Bhujangrao et al. found that in nickel-based superalloy IN718 produced by AM, more metal carbides (MC) and Laves phases appear (Figure 3 (c)). These microstructures are widely distributed in AM materials, playing a role similar to that of composite reinforcement. Finally, the AM materials achieve significantly higher hardness on the basis of sacrificing a certain degree of ductility, especially at low temperatures, as shown in Figure 4 [13]. Considering that the main working conditions of nickel-based superalloys are at relatively high temperatures, the loss of ductility is relatively small at that time, and the higher hardness brings greater performance for applications such as aircraft turbine blades. Unfortunately, although these phenomena in metal AM have been widely observed, research on more suitable mechanical models for these features is relatively scarce. Reasonable constitutive models and appropriate mechanical analysis models can effectively promote the research of metal AM materials, further improving their design and corresponding material properties, and expanding the application range of metal AM.

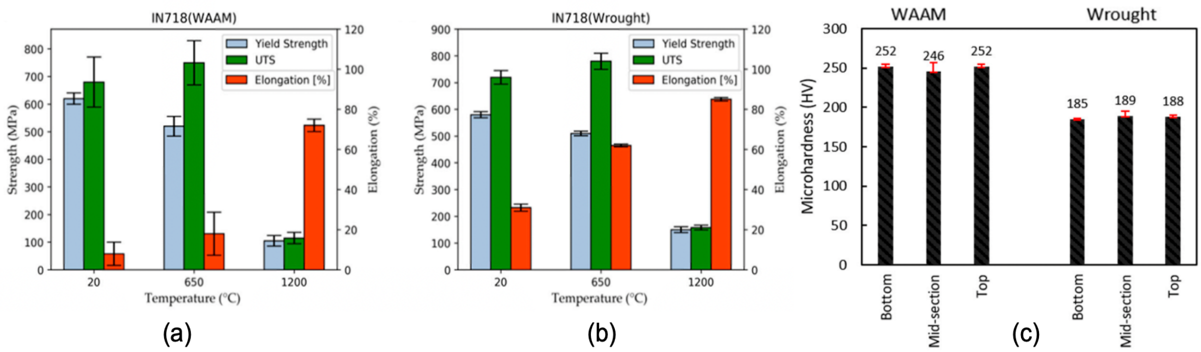

Figure 4: Strength and hardness of WAAM and wrought IN718 alloy in different temperatures and positions in the sample.

CONSTITUTIVE THEORY

In order to better characterize the material behavior at the microscale, many cross-scale constitutive models have been proposed and studied. To balance the physical mechanisms of the theory and the complexity of practical applications, the Conventional theory of Mechanism-based Strain Gradient (CMSG) and its related theory are used in this work. This theory mainly utilizes the Taylor dislocation model to correlate dislocation density with flow stress σ_{flow} and shear stress τ, as shown in the Equation (1),

$$\sigma_{flow} = M\tau \qquad \tau = \alpha\mu b\sqrt{\rho} \tag{1}$$

Combined with the relationship between total dislocation density ρ which is composed by the statistic stored dislocation density ρ_S and geometrically necessary dislocation density ρ_G, and strain gradient η^p, as shown in Equation (2),

$$\rho = \rho_S + \rho_G \qquad \rho_G = \bar{r}\frac{\eta^p}{b} \tag{2}$$

and utilizing the scale-independent and scale-dependent parts of the flow stress through uniaxial testing,

$$\sigma_{flow} = M\alpha\mu b\sqrt{\rho_S + \bar{r}\frac{\eta^p}{b}} \qquad \rho_S = \left[\frac{\sigma_{ref} f\left(\varepsilon^p\right)}{M\alpha\mu b}\right]^2 \tag{3}$$

a complete expression of the flow stress is formed, with a characteristic length l expressed by the remaining parameters, as shown in Equation (4).

$$\sigma_{flow} = \sigma_{ref}\sqrt{f^2\left(\varepsilon^p\right) + l\eta^p} \qquad l = M^2\bar{r}\alpha^2\left(\frac{\mu}{\sigma_{ref}}\right)^2 b = 18\alpha^2\left(\frac{\mu}{\sigma_{ref}}\right)^2 b \tag{4}$$

Parameters in the above equations explained as follow: M the Taylor factor, b the length of Burger's vector, α a parameter from 0.3 to 0.5, $\bar{r}$ the Nye factor, σ_{ref} a reference stress, and $f(\varepsilon^p)$ the uniaxial stress-strain function.

Combining with the traditional plastic deformation constitutive model, the final constitutive model of CMSG can describe the material size effect well, and its results are consistent with the cross-scale mechanical response of most homogeneous materials [7].

The traditional CMSG constitutive model describes the size-dependent constitutive model by introducing the size-independent result of uniaxial testing using a power-law hardening model, which has certain errors and cannot fully describe the additional size effects of materials with microscale heterostructures. Therefore, in this work, the evolution and accumulation of SSD and GND are further utilized to give a more dislocation mechanism-based constitutive relationship for flow stress in a similar form, as shown in Equation (5).

$$\sigma_{flow} = \sigma_Y + M\alpha\mu b\sqrt{\rho_{SSD} + \rho_{GND}} + \sigma_b \tag{5}$$

Each term above involves the material's initial yield stress σ_Y (related to lattice friction stress σ_0 and interfacial stress of grain boundaries σ_{GB}),

$$\sigma_Y = \sigma_0 + \sigma_{GB} = \sigma_0 + \frac{k_{HP}}{\sqrt{d}} \tag{6}$$

the evolution of SSD (related to external loading and current dislocation density),

$$\frac{\partial \rho_{SSD}}{\partial \varepsilon^p} = M\left(\frac{k_1}{bd} + \frac{k_2}{b}\sqrt{\rho_{SSD} + \rho_{GND}} - k_3\left(\frac{\dot{\varepsilon}^p}{\dot{\varepsilon}_0}\right)^{-\frac{1}{n_0}}\rho_{SSD} - \left(\frac{d_c}{d}\right)^2\rho_{SSD}\right) \tag{7}$$

the accumulation of GND (consistent with CMSG theory, the short-range effect of GND),

$$\rho_{GND} = \bar{r}\frac{\eta^p}{b} \tag{8}$$

and the additional hardening effect of back stress σ_b (related to the long-range effect of GND, i.e., gradient of the GND density).

$$\sigma_b = \frac{\sqrt{3}}{8}\frac{\mu b R^2}{(1-\nu)}\sqrt{\left(\frac{\partial \rho_{GND}}{\partial x}\right)^2 + \left(\frac{\partial \rho_{GND}}{\partial y}\right)^2 + \left(\frac{\partial \rho_{GND}}{\partial z}\right)^2} \tag{9}$$

Parameters in the above equations explained as follow: k_{HP} the Hall-Petch constant, d the diameter of the grain, R the radius of the GND affected zone, $k_1, k_2,\ k_3$ the geometric/proportionally/recovery factor, n_0 and $\dot{\varepsilon}_0$ the recovery factors, and d_c a reference grain size.

Based on these expressions and corresponding parameters, a more comprehensive constitutive model can be constructed to describe metal AM materials with microscale heterostructures, which are the focus of the present work [14]. All the simulation work on metal materials with microscale heterostructures in this work is based on the constitutive models above that takes into account the strain gradient effect. The simulations were conducted using ABAQUS and its UMAT subroutines. The meshes in all simulations have reached mesh convergence.

RESULT AND DISCUSSION

In order to simulate the typical difference between metal materials produced by AM and conventional method, namely the quantity of microscale heterogeneities, this paper employs 3D model to simulate a specific form of biphasic metal materials consisting of coarse-grained and fine-grained domains of the same/different material types, as shown in the Figure 5. Such materials can be manufactured through both conventional manufacturing processes and AM technologies.

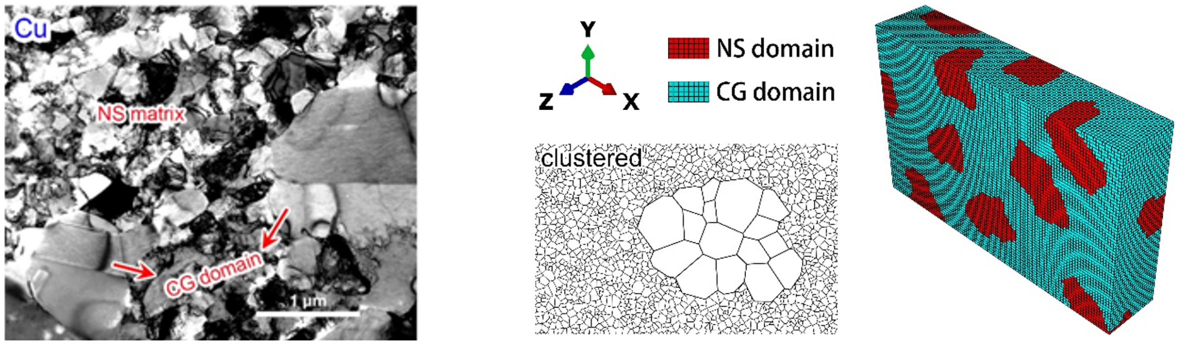

Figure 5: Two-phase metal sample and its finite element model.

In uniaxial tension tests, the change of Mises stress due to the heterogeneity in the material can be observed by controlling the presence or absence of GND in the numerical model. This helps to investigate the stress variation caused by heterogeneities at both macroscopic scales (without considering GND effect) and microscopic scales (with GND effect considered), as shown in Figure 6(c)-(e). Additionally, the extent of stress variation and width of the variation region at different size scales and strain levels in the two domains of the material can be analyzed (Figure 6(f1)-(F3)), this region is named as the hetero-zone boundary affected region (HBar). It is found that the stress change in Hbar is significant only if the GND effect (both short-range and long-range) is considered.

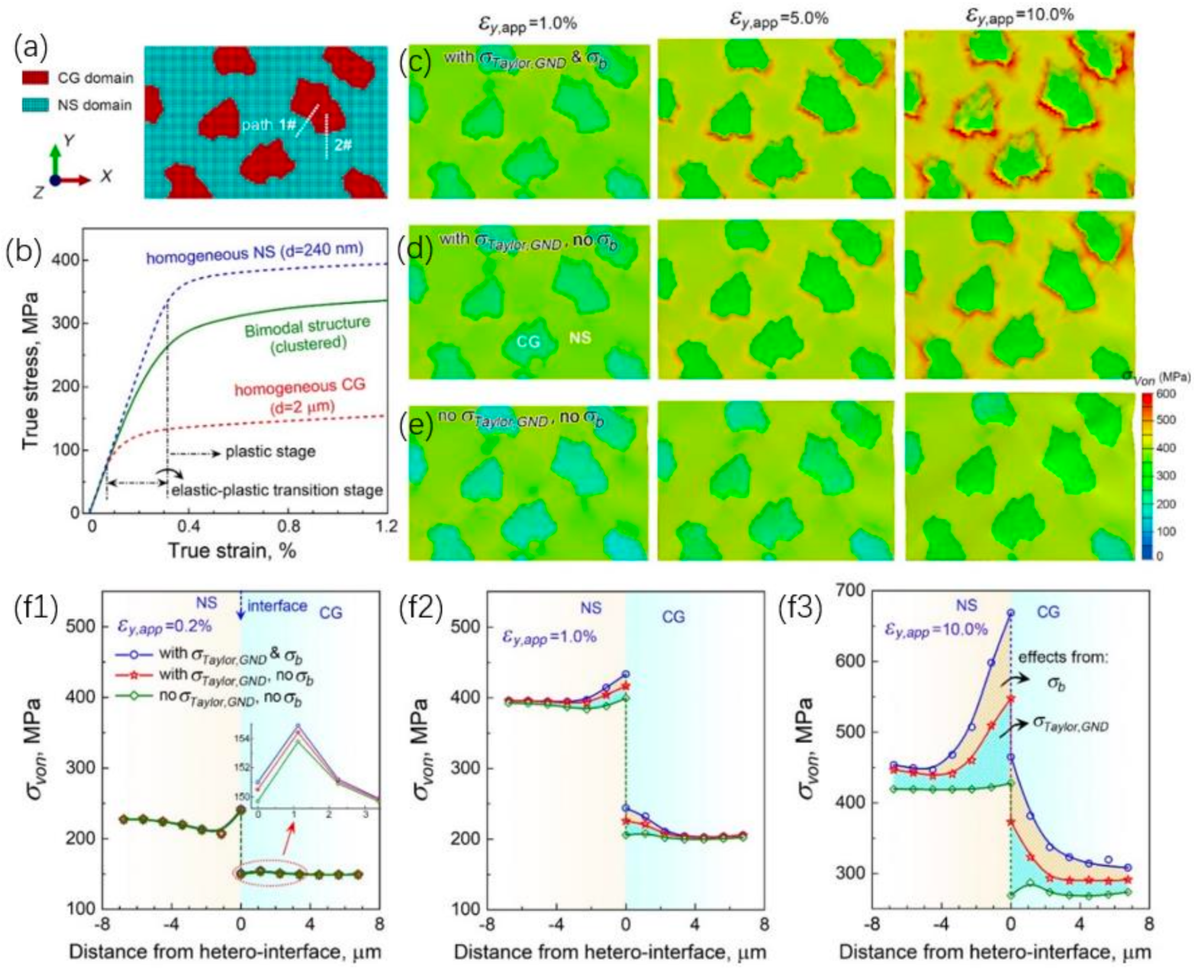

Figure 6: Stress and strain of the heteromaterial and the distribution near the domain boundary.

Strain gradient is the best manifestation of the size effect in metal AM materials at the microscale, according to the Taylor dislocation model. The distribution of strain gradient at different strain conditions is presented in Figure 7(a). It can be observed that regions with high strain gradient are almost strictly near Hbar (Figure 7(b), 7(c)), and the width of Hbar is independent of the external load (Figure 7(d)) and position (Figure 7(e)). This implies that for AM metal materials with many heterogeneities, sufficient areas with a great amount of GND will be generated under large external loads, significantly enhancing the flow stress of the material. Thus, the mechanical performance of metal components manufactured using AM technology can be improved. However, these heterogeneities are prone to cause local stress concentration, and many grain boundaries and domain interfaces are inside, which may ultimately lead to failure such as fatigue or crack propagation under large loads. Therefore, the ductility of AM metal materials will be significantly lower than those of materials produced by traditional methods if not subjected to sophisticated post-processing.

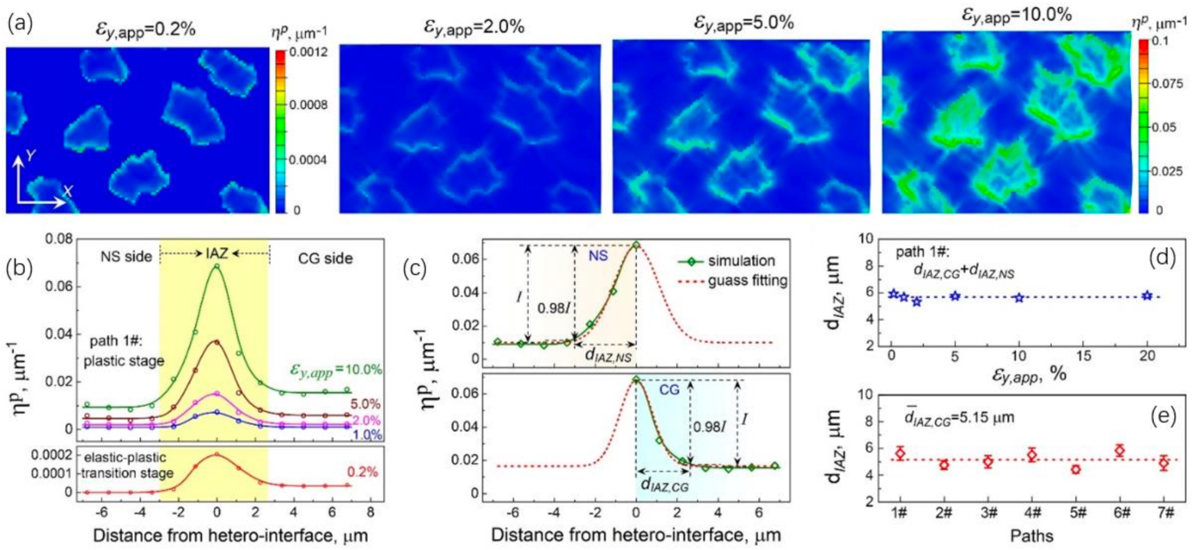

Figure 7: Distribution of strain gradient and the width of the hetero-zone boundary affected region.

The additional strength and ductility of metal AM materials mainly come from the extra hardening effect caused by GND and its gradient from the present research, thus the material's ability to withstand greater stress can be further improved by increasing the differences between the two phases in the material's heterostructure. This leads to greater non-uniform deformation near the interface, resulting in higher GND density and corresponding gradients, as shown in Figure 8 [15]. In metal AM, this can be achieved by controlling the processing conditions generate more heterostructures, methods including but not limited to the control of printing speed, temperature and metal powder properties. Also, using advanced multiphase 3D printing technologies to design and fabricate the desired heterostructures can further enhance metal material's performance.

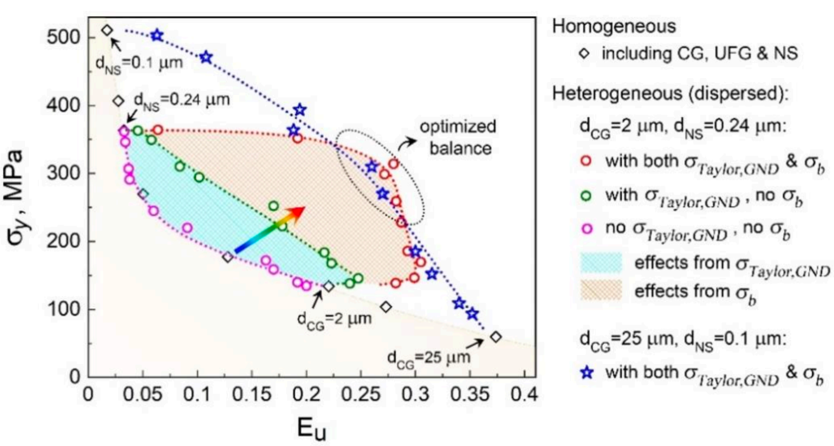

Figure 8: Relation of strength and ductility of heteromaterials with different phases.

CONCLUSION AND PROSPECT

This study is a fundamental research on materials with microscale heterogeneous structures fabricated using additive manufacturing and similar methods. The relationship between the mechanical performance of this type of material and its microstructure has been identified, and it has been suggested that the density and gradient of GND and its short- and long-range effects may be the reasons behind this particular mechanical performance. Possible methods for further improving the overall mechanical properties of materials by controlling the distribution and differences of the heterostructures in the material have been proposed. However, most structural failures in practical engineering occur before the actual plastic limit due to reasons such as fracture and fatigue. To better propose theories and simulation methods aimed at enhancing the service performance of metal additive manufacturing materials, future research will focus on the techniques to achieve such heterostructure control, and the fatigue and damage tolerance of these materials with such microscale heterostructures. These advanced metal materials, produced using additive manufacturing, will find expanded applications in critical fields like aeronautics and aerospace structures.

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