

序构纳米孪晶金属的设计及塑性变形

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摘 要: 基元序构强韧化策略为突破传统金属材料强度-塑性之间的倒置关系提供了全新思路。纳米孪晶铜因其微观结构稳定、尺度精准可调控, 以及塑性变形过程中位错机制明晰, 成为构筑序构材料、揭示其力学性能强韧化原理的理想模型。本文基于序构纳米孪晶铜的研究现状, 系统阐述层状与梯度 2 种典型序构方式对力学性能、梯度变形行为与塑性变形机制的影响规律, 旨在揭示基元序构方式调控力学性能的内在机制。此外, 本文还梳理了该领域当前面临的机遇与挑战, 以期为高性能金属材料的发展提供参考。

关键词: 基元序构金属; 纳米孪晶; 梯度与层状; 强度和塑性; 几何必需位错

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金属材料作为支撑现代工业体系的核心结构材料, 其强度、塑性等力学性能直接决定了重大装备与关键工程的服役能力与安全边界。传统金属材料的强化策略长期遵循“合金化、均匀化、均质化、纳米化等”的经典设计范式, 主要以晶粒及各种缺陷(如位错、第二相、孪晶界)为基本单元, 其核心思路是通过增加位错运动的阻力实现强化, 但是这严重限制了位错进一步储存, 发生应变局域化, 导致其塑性急剧下降^[1-3]。这种强度与塑性“鱼与熊掌难以兼得”的矛盾^[4-6]已成为制约高性能金属材料发展的重大科学挑战。

近年来, 基元序构强韧化策略为高性能金属材料的发展带来全新思路^[7-12]。基元序构金属中, 基元指构成金属中固有的基本结构单元, 如晶粒^[13-15]、缺陷(位错^[16]、孪晶^[17-19]、析出相^[20-21])等, 或二者的有效组合。序构指将不同大小、不同种类的基元在空间重新排列, 形成梯度^[13-14, 16, 22-23]、层状^[24-27]、周期分布等。与传统均匀化设计理念不同, 基元序构研究范式摒弃了单纯追求高密度、缺陷均匀分布

的做法, 转而通过精确调控跨尺度微观缺陷的空间梯度排列, 实现了从纳米到微米、毫米, 甚至更大尺度(跨越 3~7 个数量级)的多级序构协同优化。这种跨尺度、非均匀的梯度序构设计, 不仅有效避免了传统金属中常见的应变局域化问题, 更通过各基元间的协同效应, 实现了材料综合性能的非线性提升。

基元序构金属的强韧化机制与塑性应变梯度所引发的几何必需位错密切相关。序构金属材料中基元的力学响应存在显著的非同步性, 且各基元间存在强相互约束。根据应变梯度塑性理论^[28], 不均匀变形和强约束引起的塑性应变梯度及塑性变形不兼容性会导致额外几何必需位错产生: 约束愈强, 应变梯度愈大, 几何必需位错密度也愈高。大量的实验结果也已经证实, 通过增加结构梯度大小^[22]、改变梯度顺序^[29]、增加梯度层占比^[30]、优化基元占比^[25]等序构策略均可增强梯度塑性变形, 进而产生更多的几何必需位错。这些几何必需位错不仅能够通过阻碍位错运动产生额外强化, 还能增加位错储存, 提升应变硬化, 从而使材料获得良好的塑性。

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利用直流电解沉积技术制备的均匀纳米孪晶结构^[17](HNT)已得到广泛研究。该结构具有微观结构稳定、晶粒尺寸及孪晶片层厚度、取向等精准可控等特点。尤为重要的是, 纳米孪晶铜在塑性变形过程中的位错机制较为明晰^[31], 使其成为研究序构金属材料关键科学问题的理想模型基元。例如, 通过梯度纳米孪晶铜^[22, 30, 32]的研究, 量化了结构梯度大小(单位样品厚度内的硬度变化)对力学性能的影响, 揭示了梯度序构带来的额外强化效应, 并建立了涵盖结构梯度、塑性应变梯度、几何必需位错、背应力/有效应力与宏观力学性能的统一力学框架。在此基础上, 进一步阐明了梯度顺序与基元应变硬化能力对梯度纳米孪晶铜力学性能的作用规律及其内在机制。类似地, 通过设计一系列层状纳米孪晶结构^[25, 33], 明确基元厚度、体积分数及其力学性能差异对材料宏观力学性能与变形机制的影响规律。

本文重点综述梯度与层状纳米孪晶结构研究中的重要实验进展, 定量对比这 2 种序构方式对力学

性能(包括强度、塑性与应变硬化)及变形行为的影响规律, 探讨其内在科学原理, 系统阐明序构方式在实现金属材料高强度与高塑性协同提升中的关键作用。同时, 结合当前基元序构设计所面临的科学与技术挑战, 对高性能基元序构金属材料的未来发展进行了展望。

1 序构方式对力学性能的影响

1.1 层状纳米孪晶铜的微观结构与力学性能

采用直流电解沉积技术制备了层状纳米孪晶(LNT)铜样品^[25, 33]。如图 1a1~图 1d2 所示, LNT Cu 由硬基元 HNT-Ⓐ和软基元 HNT-ⓓ组成, 二者均为典型纳米孪晶结构: 晶粒呈柱状, 平均晶粒尺寸(沿短轴方向)分别为 2.5 μm 与 15.8 μm ; 晶粒内部存在高密度的孪晶界, 垂直于生长方向(样品厚度)择优分布, 孪晶片层厚度处于纳米量级, 平均值分别为 29 nm 与 72 nm。其中, 样品 LNT-200 的芯部为软基元ⓓ, 厚度为 200 μm , 两表面为硬基元Ⓐ, 厚度

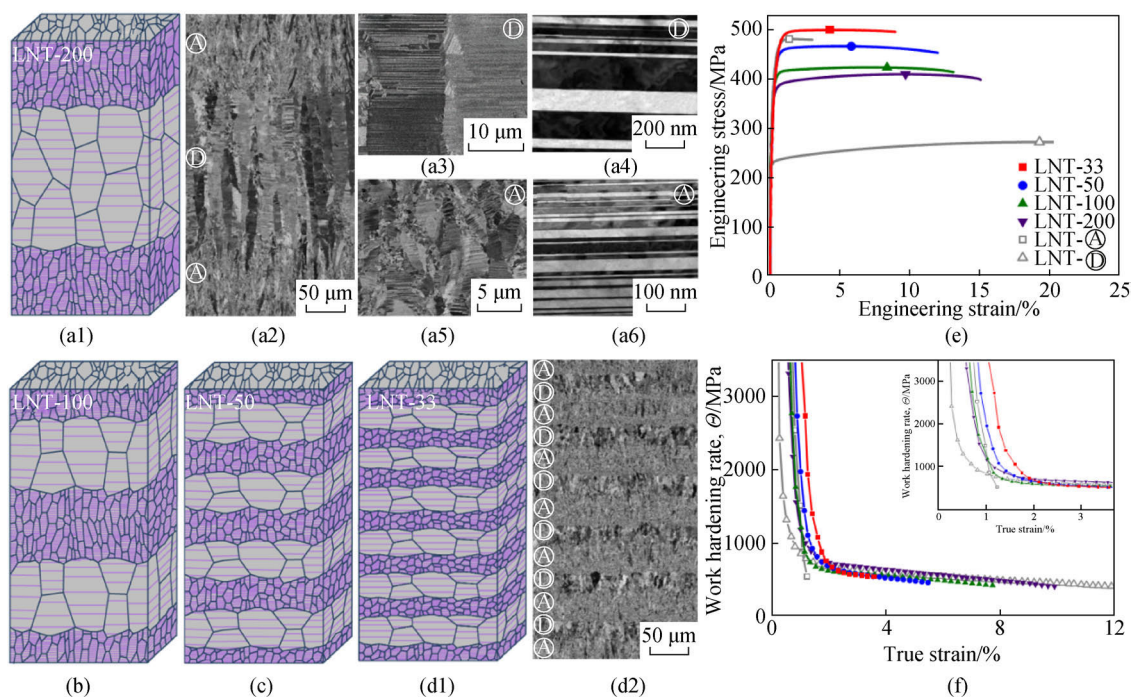


图 1 层状纳米孪晶结构(LNT)Cu 的微观结构与力学性能。(a1 和 a2)分别为样品 LNT-200 的结构示意图和横截面扫描电子显微镜(SEM)照片。(a3~a6)分别为基元ⓓ(a3 和 a4)和基元Ⓐ(a5 和 a6)的高倍 SEM 照片与透射电子显微镜(TEM)照片。(b~d1)分别为样品 LNT-100(b)、样品 LNT-50(c)和样品 LNT-33(d1)的结构示意图。(d2)为样品 LNT-33 的横截面 SEM 照片。(e~f)为 LNT Cu 与 HNT-Ⓐ和 HNT-ⓓ的拉伸工程应力-应变曲线(e)和应变硬化速率 θ -真应变曲线(f)。(f)中的插图应为应变硬化曲线在小应变下的放大图^[25]

Fig. 1 Microstructure and mechanical properties of laminated nanotwinned (LNT) Cu. The schematic (a1) and cross-sectional scanning electron microscopy (SEM) image (a2) of LNT-200 sample. High-magnification SEM (a3 and a5) and transmission electron microscopy (TEM, a4 and a6) of component ① (a3 and a4) and ② (a5 and a6). The schematic of LNT-100 (b), LNT-50 (c) and LNT-33 (d1) samples with SEM image of LNT-33 sample (d2). Engineering tensile stress-strain curves (e) and work hardening rate θ -true strain curves (f) of LNT Cu compared with HNT-Ⓐ and HNT-ⓓ. The inset of (f) shows the magnified work hardening curves at small strains ^[25]

均为 100 μm , 相邻基元间界面清晰, 形成自下而上 ①④① 的排列。样品 LNT-100、样品 LNT-50 与样品 LNT-33 分别具有 2、4、6 周期的 ①④① 基元排列, 界面间距分别为 100、50、33 μm 。

室温拉伸性能结果表明, 硬基元 HNT-① 的屈服强度较高(446 MPa), 均匀延伸率仅为 1.6%; 相反, 软基元 HNT-④ 的屈服强度较低(221 MPa), 均匀延伸率高达 21.7%, 二者呈现典型强度-塑性此消彼长的关系(图 1e)。样品 LNT-200 的屈服强度为 366 MPa, 略高于两基元的混合法则的计算值(即基元 ① 和 ④ 屈服强度的平均值), 呈现出“1+1>2”的额外强化效应。随着界面间距由 200 μm 减小至 33 μm , LNT Cu 的屈服强度逐渐增加, 塑性则相应降低。尤其是, 界面间距最小的样品 LNT-33 屈服强度高达 450 MPa, 甚至超过了最强基元 ① 本身的强度; 同时其均匀延伸率和断裂延伸率仍分别保持在约 3% 和 9%, 表现出显著的额外强韧化效应。

图 1f 展示了 HNT Cu 和 LNT Cu 的应变硬化行为, 两者均呈现典型的两阶段特征: 弹-塑性转变阶段(阶段 I)中, 即由 ① 到 ④ 的完全弹性变形逐渐到完全塑性变形的阶段, 应变硬化速率随着应变的增加迅速下降; 进入稳定塑性变形阶段(阶段 II)后, 下降速率明显减缓。对于单一基元, HNT-① 在阶段 I 具有较高的应变硬化速率, 但无阶段 II; HNT-④ 在阶段 I 的应变硬化速率较低, 但阶段 II 持续较长。层状样品中, 样品 LNT-200 在阶段 I 的应变硬化速率接近于 HNT-①。随着界面间距从 200 μm 减小至 33 μm (图 1f 插图), LNT Cu 在阶段 I 的应变硬化程度显著增加, 这与屈服强度的提高趋势一致。然而, 在大应变下, LNT Cu 的应变硬化速率略有降低, 表明其额外应变硬化主要源于初始变形阶段。

具体来说, 在变形初期, 所有基元均为弹性变形; 随着应变增加, 屈服强度最低的基元 ④ 率先发生塑性变形, 而其他基元强度仍处于弹性变形阶段; 后续, 剩余基元依次发生塑性变形; 屈服强度最高的基元 ① 最后发生塑性变形。这种由软基元到硬基元非同步、渐进式的弹-塑性变形转变形成了由基元 ① 到 ④ 梯度增加的塑性应变。根据经典的应变梯度塑性理论^[28], 为协调这种塑性应变梯度带来的晶格非完整、非连续性, 必须产生额外的几何必需位错, 当几何必需位错的密度足够高时, 便可贡献显著的额外强化和额外应变硬化。因此, 应变硬化阶段 I 的发生, 即弹-塑性转变阶段, 对实现序构金属的额外强化与加工硬化至关重要。

1.2 梯度纳米孪晶铜的微观结构与力学性能

与层状纳米孪晶结构不同, 梯度纳米孪晶(GNT)结构由 4 个 HNT 基元(①、②、③和④)构成, 如图 2a1~图 2d2。从基元 ① 到 ④, 晶粒尺寸与孪晶片层厚度逐渐增大^[22]。样品 GNT-1 采用基元 ①、②、③ 到 ④ 自下而上的顺序排列, 形成了单向梯度结构; 样品 GNT-2 则按通过 ①②③④③②① 的顺序排列, 实现了对称梯度分布。在此基础上, 进一步分别设计了具有 2 和 4 周期 ①②③④③②① 排列的样品 GNT-3 和样品 GNT-4。为定量表征 GNT Cu 的梯度结构特征, 将单位厚度内硬度的变化定义为结构梯度。由样品 GNT-1 到样品 GNT-4, 样品总厚度、各基元的体积分数均保持不变, 结构梯度由 1.75 GPa/mm 增加到 11.6 GPa/mm, 实现了结构梯度的可控调节。

室温拉伸性能结果表明, 与 HNT Cu 相比, GNT Cu 具有更高的强度和应变硬化速率, 表现出更加显著的“1+1>2”额外强化与应变硬化行为。如图 2e 所示, 由样品 GNT-1 到样品 GNT-4, 随结构梯度增加, GNT Cu 的屈服强度从 364 MPa 增加至 481 MPa, 与此同时, 其均匀延伸率基本保持不变。当结构梯度达到 11.6 GPa/mm 时, 样品 GNT-4 的屈服强度甚至超过了梯度孪晶结构中强度最高的基元 ①(446 MPa), 且仍保持约 7% 的均匀延伸率, 即实现了高强度和高塑性的协同提升。不仅如此, 所有 GNT 样品的应变硬化速率均高于应变硬化率最高的基元 ④, 呈现出显著的额外应变硬化效应(图 2f)。尤其是在小应变(~1%)下, GNT Cu 的应变硬化率随结构梯度显著增加, 这与屈服强度的提高趋势一致。这种独特的由结构梯度引起的额外强韧化行为在其他结构材料中均未观察到^[13, 19, 34, 35]。

1.3 层状与梯度纳米孪晶铜的力学性能对比

图 3a 总结了 LNT Cu 与 GNT Cu 的额外强化随结构梯度的变化规律, 其额外强化定义为:

$$\Delta\sigma = \frac{\sigma_y - \sigma_y^{\text{ROM}}}{\sigma_y^{\text{ROM}}} \quad (1)$$

其中: σ_y 为 LNT Cu 或 GNT Cu 的屈服强度; σ_y^{ROM} 为对应的混合法则强度(各基元强度的平均值)^[36]。对于 LNT Cu, 当界面间距由 200 μm 减少至 33 μm 时, 其等效结构梯度(即软硬基元硬度差与二者中心的距离之比)由 1 GPa/mm 增加到 19.7 GPa/mm, 其额外强化由 3.6% 增大到 34.7%。对于 GNT Cu, 当结构梯度由 1.75 GPa/mm 增加到 11.6 GPa/mm 时, 其额外强化由 4.6% 增加至 38.6%, 明显高于

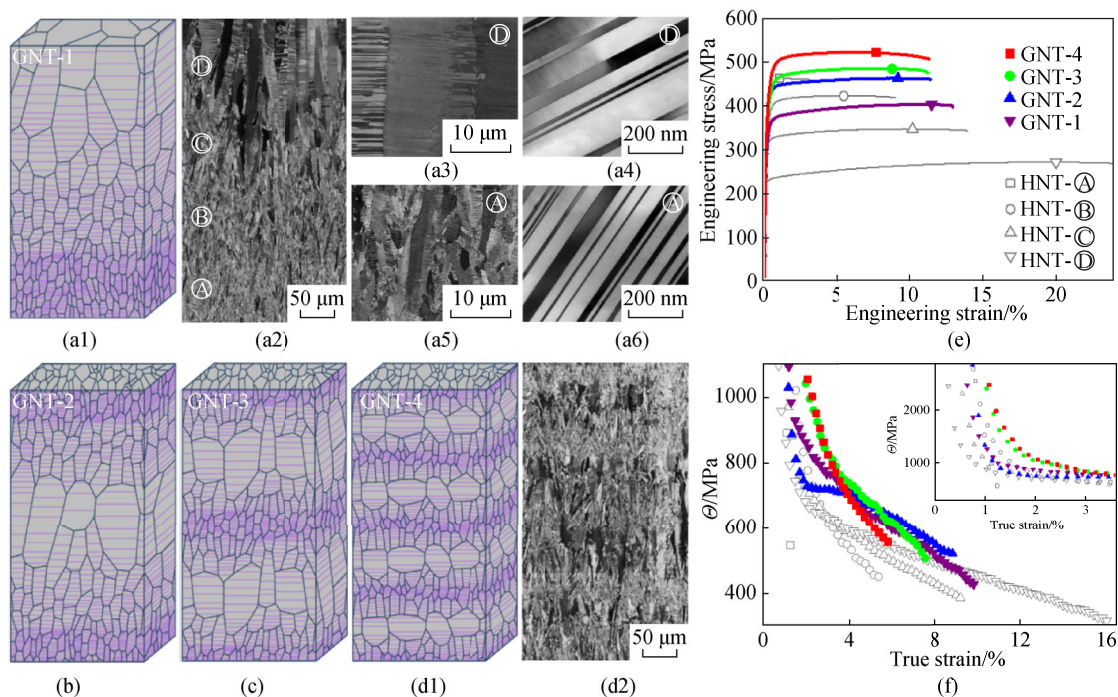


图2 梯度纳米孪晶结构(GNT)Cu的微观结构与力学性能。(a1和a2)分别为样品GNT-1的结构示意图和横截面SEM照片。(a3~a6)分别为基元①(a3和a4)和基元②(a5和a6)的高倍SEM照片与TEM照片。(b~d1)分别为样品GNT-2(b)、样品GNT-3(c)和样品GNT-4(d1)的结构示意图。(d2)为样品GNT-4的横截面SEM照片。(e~f)为GNT Cu及其均匀组元HNT Cu的拉伸工程应力-应变曲线(e)和应变硬化速率 θ -真应变曲线(f)。(f)中的插图为应变硬化曲线在小应变下的放大图^[22]。

Fig. 2 Microstructure and mechanical properties of gradient nanotwinned (GNT) Cu. The schematic (a1) and cross-sectional SEM image (a2) of GNT-1 sample. High-magnification SEM (a3 and a5) and TEM (a4 and a6) of component ① (a3 and a4) and ② (a5 and a6). The schematic of GNT-2 (b), GNT-3 (c) and GNT-4 (d1) samples with SEM image of GNT-4 (d2). Engineering tensile stress-strain curves (e) and work hardening rate θ -true strain curves (f) of GNT Cu compared with freestanding HNT Cu samples. The inset of (f) shows the magnified work hardening curves at small strains^[22]

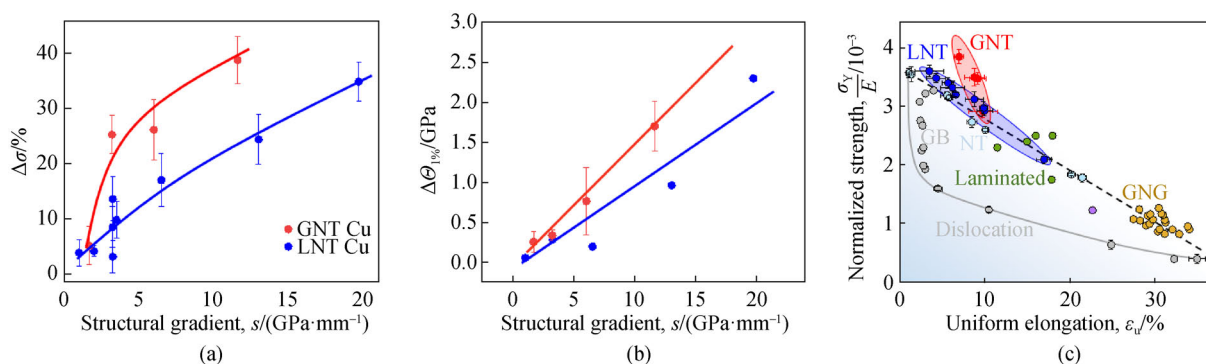


图3 GNT Cu和LNT Cu的(a)额外强化 $\Delta\sigma$ 和(b)真应变为1%时的额外应变硬化率 $\Delta\theta_{1\%}$ 与结构梯度的关系。(c)GNT Cu归一化屈服强度(σ_y/E , E 为弹性模量)与均匀延伸率关系图。为了对比,还包括了传统的强化方式比如位错(dislocation)^[37]、细晶强化(GB)^[38-39]、纳米孪晶(NT)^[17]、层状结构(laminated)^[40]和梯度纳米晶(GNG)^[13, 34]

Fig. 3 (a) Extra strengthening $\Delta\sigma$ and (b) extra work hardening rate at 1% true strain $\Delta\theta_{1\%}$ versus structural gradient (s) of GNT and LNT Cu. (c) Yield strength normalized by Young's modulus versus uniform elongation of GNT Cu samples, in comparison with metals and alloys strengthened by dislocations^[37], grain boundaries (GBs)^[38-39], highly oriented nanotwins^[17], laminated and gradient nanograined (GNG) structures^[13, 34]

LNT Cu 中额外强化随结构梯度增加的程度,说明梯度序构比层状序构更有助于提升额外强化。

类似地,图3b对比了LNT Cu与GNT Cu在变形初期额外应变硬化随结构梯度的变化规律,其中

额外应变硬化被定义为:

$$\Delta\theta = \frac{\theta_{1\%} - \theta_{1\%}^{\text{ROM}}}{\theta_{1\%}^{\text{ROM}}} \quad (2)$$

其中: $\theta_{1\%}$ 为 LNT Cu 或 GNT Cu 在真应变量为 1% 的应变硬化率; $\theta_{1\%}^{\text{ROM}}$ 为对应的混合法则应变硬化率(各基元应变硬化率的平均值)。很明显, 当结构梯度大小相当时, GNT Cu 相较于 LNT Cu 表现出更高的额外应变硬化, 表明梯度序构具有比层状序构更强的应变硬化能力。

图 3c 总结 LNT Cu 与 GNT Cu 以及其他均匀或非均匀结构金属材料的强度-塑性。相比于传统金属材料所呈现的显著强度与塑性倒置, 具有纳米孪晶结构、层状纳米晶结构与梯度纳米晶结构的金属材料在强度-塑性匹配上已有明显改善, 但大多仍遵循“1+1=2”的混合法则(如黑色虚线所示)^[36]。层状纳米孪晶结构的强度-塑性得到一定提升, 尤其是在高强度水平下仍能保持一定塑性^[25]。而梯度纳米孪晶结构则实现了强度-塑性的进一步的协同提升, 其综合性能完全超越了现有均匀或非均匀结构的典型范围, 突破了二者严重倒置的性能瓶颈^[22]。以上结果表明, 梯度序构在优化强度-塑性综合性能方面具有更显著的优势。

2 序构方式对梯度塑性变形与位错机制的影响

普遍认为, 基元序构金属材料的额外强化与应

变硬化来源于塑性应变梯度所引发的几何必需位错^[28, 41]。在两类序构样品中, 软基元①因屈服强度较低而率先发生塑性变形, 硬基元②则因屈服强度较高而塑性变形滞后。这种渐进屈服行为使得塑性应变从硬基元到软基元逐渐增大, 形成塑性应变梯度, 进而成为几何必需位错产生的重要来源。

为定量对比层状与梯度序构方式对塑性应变梯度的影响, 利用全场应变分布技术分别测量了 LNT Cu 与 GNT Cu 的塑性应变, 拉伸样品侧表面应变分布测量示意如图 4a 所示。从图 4b2~图 4b4 可以看出, LNT Cu 在变形初期(应变 0.5%)即出现非均匀塑性变形, 其中芯部软基元①的塑性应变(ε_z)明显高于表层硬基元②, 塑性应变梯度主要集中在界面附近。随拉伸应变增加, 软、硬基元塑性应变同步增加, 界面处塑性应变梯度集中的现象持续存在。不同于 LNT Cu, GNT Cu 的塑性应变由芯部到表层逐渐、缓慢增加, 未观察到明显的塑性应变梯度集中(图 4c2~图 4c4), 表明塑性应变梯度均匀地分布在样品中。上述结果表明, 序构方式显著影响塑性应变梯度的分布特征: 在层状序构中, 塑性应变梯度主要集中于界面附近区域; 而在梯度序构中, 塑性应变梯度则弥散分布于整个样品范围^[30, 42]。

塑性应变梯度引发的几何必需位错分布及其交互作用可从微观结构中得以进一步验证。如图 5a 所示, 大量的位错在 LNT Cu 中软、硬基元界面处富集。通过采用透射电子显微镜(TEM)下的双束衍射技术, 在高倍数条件下逐根辨识位错线, 通过统

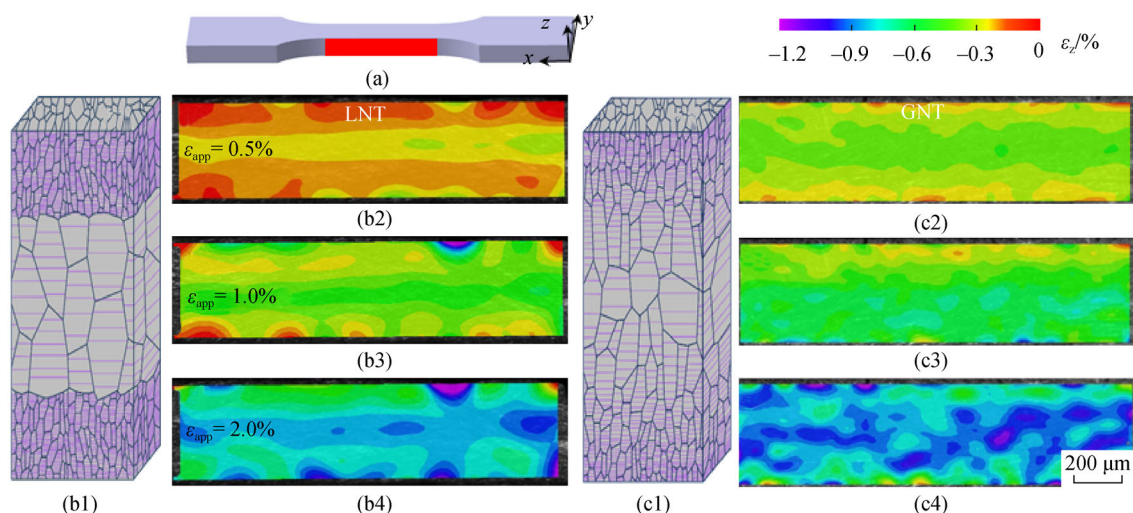


图 4 (a)拉伸试样侧表面(x - z 平面)上(红色区域)进行应变分布测量的示意图。LNT Cu(b1~b4)和 GNT Cu(c1~c4)在拉伸应变 $\varepsilon_{\text{app}}=0.5\%$ 、 1.0% 和 2.0% 时侧向应变 ε_z 的分布情况^[25, 30]

Fig. 4 (a) Schematics illustrating the strain distribution measurement on the lateral surface (x - z plane) indicated by red of tensile samples. The schematics (b1) and distribution of lateral strain ε_z of LNT Cu (b2~b4) at increasing applied tensile strain ε_{app} as indicated. (c1~c4) are same as (b1~b4) and except for GNT Cu^[25, 30]

计单位面积内的位错数量,即可获得该微区的位错密度值。通过对比界面处(1区)与远离界面处(2区)发现,大量的I类位错(位错矢量与滑移面均相交于孪晶面)在界面处富集,密度高达 $4.1 \times 10^{13} \text{ m}^{-2}$,而II类位错(位错矢量与滑移面分别平行、相交于孪晶面)密度较低,仅为 $0.8 \times 10^{13} \text{ m}^{-2}$ (图5b~图5d)。相反,2区(图5e~图5g)中I类位错密度较低

($0.6 \times 10^{13} \text{ m}^{-2}$), II类位错密度较高($3.0 \times 10^{13} \text{ m}^{-2}$)。实际上,由于拉伸变形过程中加载轴与孪晶方向平行,均匀纳米孪晶 HNT 样品的塑性变形仅能激发II类位错,只有在加载轴与孪晶界垂直时I类位错才会大量开动。这表明 LNT 样品中, I类位错作为额外激发的几何必需位错,用以协调界面处的塑性应变梯度^[25]。

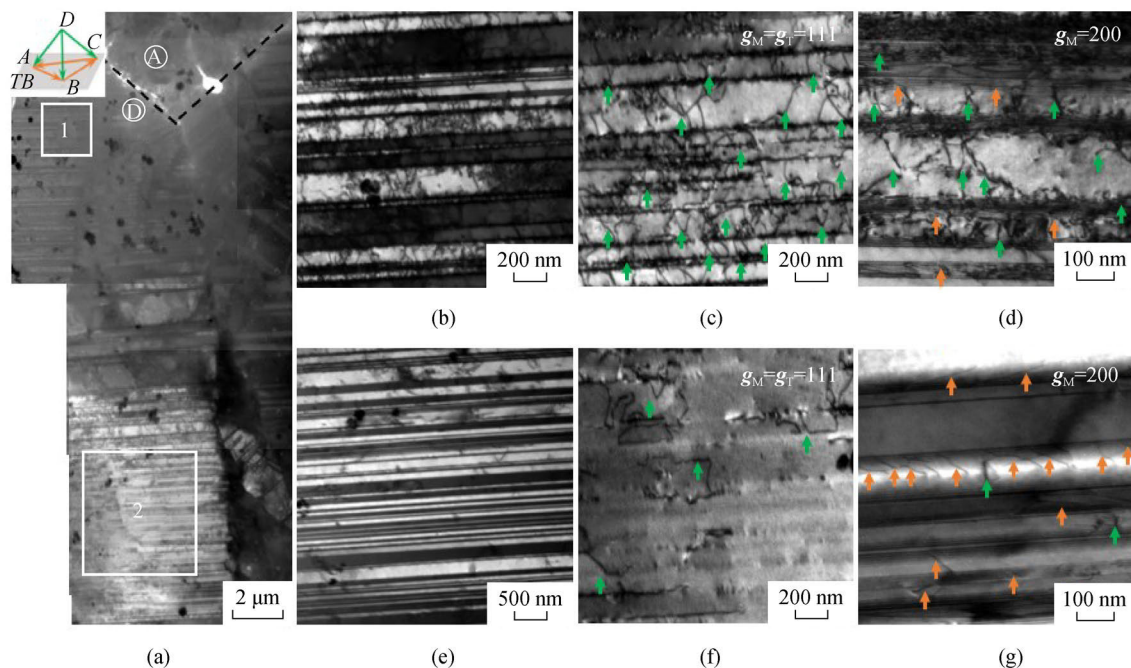


图5 拉伸应变 $\varepsilon = 3\%$ 时样品 LNT-50 靠近界面和远离界面的位错形态: 界面附近微观结构的低倍透射电子显微镜(TEM)照片(a); (b, c, d)和(e, f, g)分别为(a)中白框1和2中区域的放大照片; (c, f)和(d, g)分别为双束衍射条件下衍射矢量为 $g_M = g_T = 111$ 和 $g_M = 200$ 时的 TEM 照片。(a)中虚线指示基元A和D间的界面位置; I类位错和II类位错分别用绿色和橙色箭头指示^[25]

Fig. 5 Dislocation morphologies near and away from an interface in LNT-50 sample at $\varepsilon = 3\%$. (a) Low-magnification transmission electron microscope (TEM) image across the interface. The white rectangle region 1 and 2 in (a) are magnified into (b, c, d) and (e, f, g), respectively. (c, f) and (d, g) are imaged using two-beam diffraction with vectors of $g_M = g_T = 111$ and $g_M = 200$, respectively. The black dash line in (a) outlines the interface between component A and D. Mode I and Mode II dislocations are indicated by green and orange arrows, respectively^[25]

GNT Cu 塑性变形诱发的几何必需位错均匀地分布于各基元^[22, 42–43], 如图6a和图6b所示。大量的位错富集束结构沿着梯度方向分布, 其总位错密度较均匀基元提高了1个数量级, 高达约 10^{14} m^{-2} 。高倍双束衍射成像表明(图6b、图6c、图6e和图6f)位错富集束由大量的I类位错与少量的II类位错组成。这些I类位错不仅有效增加了总位错密度, 还能与其他位错发生交互作用, 促进位错在晶粒内部的储存, 并抑制其在晶界处的湮灭。上述观察表明, 序构方式显著影响几何必需位错的分布特征: 梯度序构使几何必需位错均匀分散于整体样品中, 并促使晶粒内部形成位错富集束。

根据应变梯度塑性理论^[28, 44], 背应力 σ_b 与几何必需位错密度 ρ_G 成正比, 可表达为:

$$\sigma_b = \beta \mu b d \rho_G \quad (3)$$

其中: β 为系数; d 为晶粒尺寸; μ 为剪切模量; b 为位错矢量^[42]。基元序构金属材料的强韧化效应主要通过几何必需位错产生长程的背应力实现。测试表明, 结构梯度相同的 LNT Cu 与 GNT Cu, 其几何必需位错密度相同, 但 GNT Cu 的背应力显著高于 LNT Cu, 该背应力主要来源于几何必需位错的分布。也就是说, 均匀分散的几何必需位错可与更多位错发生交互作用, 其长程交互的概率增大, 从而产生更高的背应力。

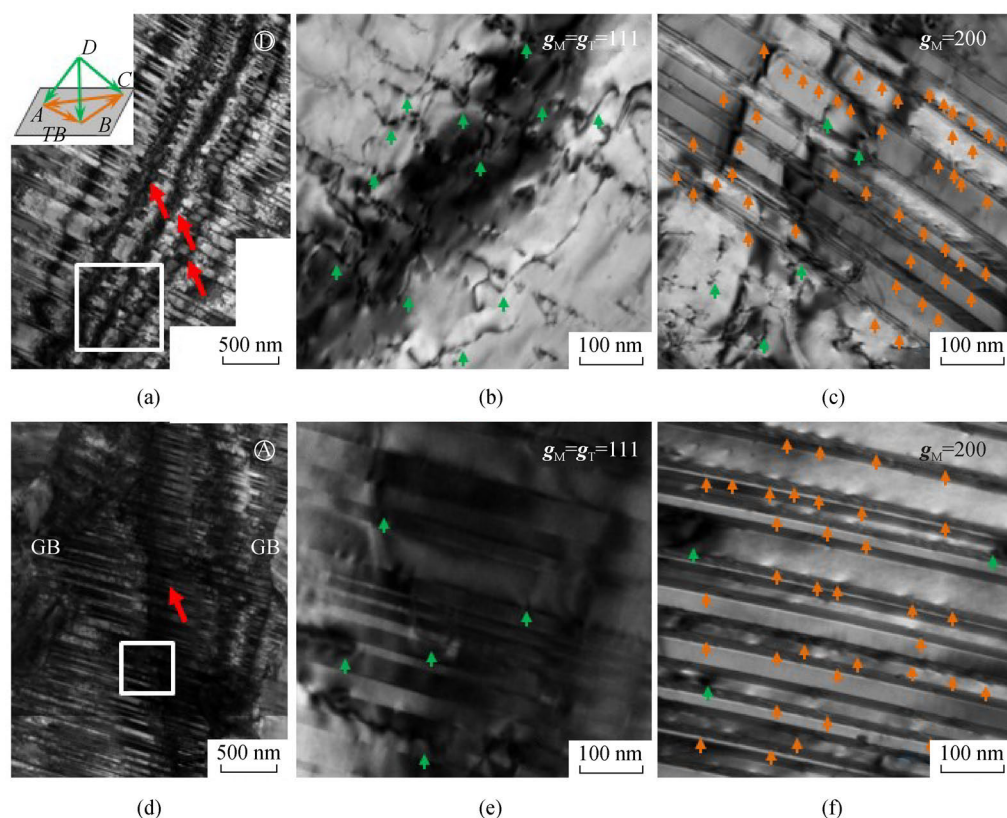


图 6 应变 $\varepsilon=1\%$ 时, GNT-4 中基元①(a~c)和②(d~f)的位错形貌。(a)和(d)为 TEM 明场像; (b, c)和(e, f)分别为(a)和(d)中白框区域的放大照片。(b)和(e)为在双束衍射条件 $g_M = g_T = 111$ 下的 TEM 位错形貌照片。(c)和(f)为在双束衍射条件 $g_M = 200$ 下的 TEM 位错形貌照片。位错富集束结构如红色箭头所示; I 类位错和 II 类位错分别如绿色和橙色箭头所示^[22]

Fig. 6 TEM images of components ① (a~c) and ② (d~f) in GNT-4 deformed at $\varepsilon=1\%$. (b and c) TEM images of the BCD region indicated by the white square in (a) identified by two-beam diffraction using vectors of $g_M = g_T = 111$ (b) and $g_M = 200$ (c), respectively. (e and f) TEM images of the BCD region indicated by the white square box in (d) identified by two-beam diffraction using vectors of $g_M = g_T = 111$ (e) and $g_M = 200$ (f), respectively. The bundles of concentrated dislocations are indicated by red arrows. Mode I and Mode II dislocations are indicated by green arrows and orange arrows, respectively^[22]

根据经典的位错塞积背应力模型^[45-46], 聚集或塞积的几何必需位错会产生屏蔽效应, 使应力场相互抵消, 从而降低总(平均)背应力。因此, 几何必需位错分布越分散, 屏蔽作用越小, 产生的背应力越强。此外, 更分散的几何必需位错增强了晶粒内部的位错交互作用, 抑制位错在晶界处的湮灭, 有助于维持较高的应变硬化率, 延缓应变局域化, 从而提升材料塑性。

3 总结与展望

本文总结了序构纳米孪晶铜的研究进展, 阐明了层状与梯度 2 种典型序构方式对其力学性能、梯度变形行为及塑性变形机制的影响规律, 并探讨了序构设计在调控金属材料强韧化行为中的作用。对比分析表明, 梯度序构能够使塑性应变梯度在样品整体范围内均匀分布, 从而激发更显著的额外强化效应与应变硬化能力, 最终实现更优的强度-塑性

匹配。

传统金属材料的微观结构尺寸通常围绕单一平均值呈统计学分布, 分布范围有限, 可近似视为均匀结构。与之不同, 基元序构材料由多种具有不同微观结构特征尺寸的基元组成, 其微观结构尺寸可跨越从纳米量级到微米量级甚至毫米量级的广阔范围, 实现了多尺度、跨层级的微观结构设计, 显著拓宽了金属材料的微观结构范围。

然而, 有关基元序构金属材料的构效关系、变革性性能及力学原理的系统研究还处于起步阶段。现有结构材料在设计、制备、表征、强韧化理论方向的全链条研究, 均建立在传统的基于均匀结构、连续介质模型的理论之上。因此, 基元序构金属材料从非均匀、跨多尺度微观结构的设计原理、制备技术、宏微观表征方法到强韧化原理、断裂力学基础理论等均面临诸多挑战。

基元序构金属的设计涉及序构参数(梯度大小、

顺序、基元占比、维度等)与基元参数(种类、组合、厚度、尺寸等)的高度复杂性与自由度,目前尚缺乏系统设计准则。探索极小结构基元、突破序构极限,是深化该方向的重要科学问题。

序构金属材料的可控制备面临的挑战更加严峻。现有的表面机械处理^[13, 21]、摩擦^[47]等塑性变形技术,仅在样品表面引入剧烈的塑性变形,形成表面梯度结构,难以实现全样品尺度的空间序构。目前,制备序构金属的可行路径主要有两种:“自下而上”的电化学沉积技术^[17]与“自上而下”的循环扭转技术^[16]。以电化学沉积为例,材料的微观结构强烈依赖于电解液温度、电流密度等工艺参数,为多类基元序构材料的制备提供了可能。然而,沉积微观结构还受到前后基元制备参数(如外延生长等)的耦合影响,显著增加了可控制备的复杂性。总之,如何通过精准调控直流电解沉积的多维工艺参数,实现具有不同组合基元与梯度序构特征(包括梯度大小、顺序、占比、线性/非线性分布、空间维度等)的金属材料可控制备,仍是当前面临的核心技术挑战。

金属材料作为承载结构件,其力学性能涵盖强度、塑性、应变硬化等基本性能,以及疲劳、断裂、蠕变等服役性能。因此,全面建立基元序构参数与力学性能之间的构效关系、澄清其力学机理,是该领域长期存在的共性科学问题。基元序构金属材料的变形机制具有高度复杂性,主要体现在两方面:其一,基元间的长程约束作用引发梯度塑性变形,产生几何必需位错等新变形载体,宏观上表现为塑性应变梯度的形成及应力状态的改变;其二,序构诱导的新载体与材料内部其他缺陷之间发生短程交互作用。目前,对基元序构约束作用内在机理的理解仍不够深入,亟须结合实验表征、力学模拟与晶体塑性理论开展协同攻关。尤其是需要发展涉及基元与序构参数耦合作用的强韧化、疲劳、断裂等相关的连续介质力学理论,以奠定该领域的理论基础。

综上所述,发展系统的基元序构构效关系与设计准则,突破精确可控制备技术,澄清基元序构增强力学性能的内在机理,进而构建从序构设计到变革性力学性能的理论与技术体系是本领域未来研究的重点。上述关键问题的突破,将为高性能金属材料的按需设计与制备提供科学依据,推动金属材料研究向更广阔的应用领域拓展。

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Design and Mechanical Properties of Metals with Ordered Units

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Extended Abstract

The strategy of units ordering offers a new approach to overcoming the conventional trade-off between strength and plasticity in metallic materials. Nano-twinned copper (Cu) serves as an ideal model system for constructing ordered materials and unraveling the mechanisms underlying their enhanced mechanical properties due to its stable microstructure, precisely controllable microstructures, and well-understood dislocation mechanisms during plastic deformation. Based on the existing research on ordered nanotwinned Cu, this review systematically elucidates the effects of two typical ordering configurations (*i.e.*, layered and gradient structures) on the

mechanical properties, deformation behavior, and plastic deformation mechanisms. The aim is to reveal the intrinsic mechanisms by which the units ordering regulates the mechanical performance. Also, this review outlines the existing opportunities and challenges in this field to provide a reference for the development of high-performance metallic materials.

The strength and ductility as critical mechanical properties of metallic materials often exhibit a trade-off relationship. This phenomenon becomes a formidable bottleneck in conventional strengthening strategies that rely on solid solution, second-phase particles, grain refinement, and dislocations, with homogeneous or randomly microstructure. Fortunately, the ordering architecture of units offers a promising pathway to overcome this limitation, attracting recent attention. Typical ordered configurations include laminated and gradient structures, where the units consist of common microstructural features such as grains, twins, dislocations, and phases. Numerous studies demonstrate that the laminated and gradient architectures both can achieve a superior combination of strength and ductility, thereby mitigating the strength–ductility trade-off. The underlying mechanism is often qualitatively attributed to heterogeneous plastic deformation across different sections and the associated formation of geometrically necessary dislocations (GNDs), promoting extra strengthening and work hardening through long-range back stress. However, a quantitative understanding of how the specific ordering strategy affects the mechanical properties, and the strengthening mechanisms remains elusive. In this review, we systematically compare the mechanical properties and deformation mechanisms of laminated nano-twinned (LNT) Cu and gradient nano-twinned (GNT) Cu to address this important issue.

LNT and GNT Cu both exhibit extra strengthening and enhanced work hardening, as demonstrated by their strengths, and the work-hardening rates at small strains exceed the corresponding rule-of-mixture predictions. These effects are further amplified *via* increasing the structural gradient, defined as the hardness variation per unit depth. GNT Cu demonstrates superior enhancements in both strength and work hardening, compared to LNT Cu, highlighting the advantage of gradient ordering over laminated ordering. Compared to conventional homogeneous or randomly heterogeneous structures, LNT and GNT architectures both achieve an enhanced strength–ductility synergy. In particular, the GNT structure maintains a considerable ductility with only a minor reduction as the strength increases. GNT Cu with the maximum structural gradient exhibits strength exceeding that of its strongest constituent unit, while retaining appreciable ductility. These results demonstrate that gradient ordering can induce stronger strengthening and superior strength–ductility synergy, compared to laminated ordering.

LNT and GNT Cu both display a characteristic gradient plastic deformation across their sections, which promotes the accumulation of GNDs and thereby enhances strengthening and work hardening. In LNT Cu, plastic strain gradients and GNDs concentrate mainly at interfaces. In contrast, in GNT Cu, they are distributed more homogeneously throughout all thesections, forming bundles of concentrated dislocations within grain interiors. Consequently, the dislocation density in GNT Cu is nearly an order of magnitude higher than that in its homogeneous counterparts. Moreover, these dispersed GNDs interact more frequently with other dislocations, generating higher back stresses, compared to the interface-accumulated GNDs in LNT Cu. This GND-distribution-dominated strengthening mechanism is responsible for the superior strength–ductility synergy achieved through gradient ordering.

Summary and Perspects This review systematically compares the mechanical properties and deformation mechanisms of LNT and GNT Cu to elucidate the quantitative effect of ordering strategy on the performance. Gradient ordering can provide greater extra strengthening and work hardening than laminated ordering, leading to a superior strength–ductility synergy. The underlying mechanism is rooted in the distinct distribution of plastic strain gradients and GNDs, while laminated ordering leads to GND accumulation at interfaces, gradient ordering promotes their dispersion throughout all the sections. These dispersed GNDs contribute to stronger strengthening and work hardening *via* enhanced back stress generation.

Despite recent advances on unit-ordering metallic materials, systematic research on their structure–property relationships and associated mechanisms remains in its early stages. This is particularly true for establishing design criteria for unit-ordering strategies that optimize the performance including strength, ductility, fatigue and fracture resistance, considering the complicated ordering and unit parameters such as ordering way, structural gradient, ordering sequence, unit type and their proportions. More importantly, it remains a challenge to fully understand the deformation mechanism of unit ordering metals, especially in the long-range inter-constraint across sections, which plays an important role in producing the deformation carriers for gradient deformation and extra strengthening. It is encouraged to combine experimental characterization, simulation, and mechanics modelling to address the key issues above.

Keywords metallic materials with unit ordering; nanotwins; laminated and gradient; strength and ductility; geometrically necessary dislocations