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# Expanding the Design Space of Nb–Ti–Al-Related Lightweight Alloys: From High-Nb TiAl Intermetallics to Zr–Ti–Nb–(Al)-Concentrated BCC Matrices

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**Abstract**

Nb-containing TiAl alloys are among the most important lightweight intermetallics for high-temperature applications because they combine low density with useful strength, oxidation resistance and creep resistance. Their long-standing difficulty is equally clear: the ordered $\gamma/\alpha_2$ matrix and lamellar hierarchy that support thermal stability also restrict plastic accommodation and manufacturing tolerance. This Perspective addresses a specific question: how can Nb–Ti–Al-related alloy design expand from stabilizing ordered TiAl matrices toward matrices and architectures that also enable scalable deformation and processing? The discussion is organized around three connected routes. High-Nb TiAl alloys established a durable service-stability platform; lamellar, colony, and orientation engineering then created deformation pathways within ordered matrices, and compositionally adjacent Zr–Ti–Nb–(Al)-concentrated BCC alloys introduced a different matrix-selection strategy in which chemical disorder and BCC stability are used to build processability at an earlier stage of design. These routes solve different parts of the same design problem rather than representing direct competitors. They indicate that future lightweight high-temperature alloys should be designed by linking composition selection, phase architecture, thermomechanical processing and environmental validation within a processability–stability framework.

**Keywords:** Nb–Ti–Al-related lightweight alloys; high-Nb TiAl; concentrated BCC alloys; medium-entropy alloys; matrix selection; processability–stability co-design

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## 1. Introduction

Lightweight structural materials for aero-engines, transportation and energy systems must retain load-bearing capacity at temperatures where conventional titanium alloys lose strength, while nickel-based superalloys increase component weight because of their higher density. γ-TiAl-based intermetallics occupy a distinctive position in this landscape. Their low density and useful high-temperature properties made them attractive for rotating components, and the commercial use of TiAl blades demonstrated that ordered intermetallics can move from laboratory alloys to engineered components when composition, processing and design are coordinated [1,2].

The central obstacle has remained almost unchanged. The same ordered bonding and lamellar hierarchy that give $\gamma/\alpha_2$ TiAl alloys high-temperature stability also restrict slip transfer, crack-tip plasticity and room-temperature workability [3]. In practice, TiAl

alloy design has therefore been shaped less by a single target property than by a persistent negotiation between service stability and plastic accommodation [4]. The history of Nb-containing TiAl is one important response to this negotiation. Nb additions improved the high-temperature relevance of TiAl by strengthening the ordered matrix, modifying phase stability, and improving environmental resistance [5].

Yet the broader development of Nb–Ti–Al-related lightweight alloys did not stop at stabilizing an ordered TiAl matrix. Once high-Nb TiAl had become a credible service platform, increasing attention moved toward the architecture of deformation: colony size, lamellar spacing, twins, interfaces, texture and orientation. More recently, Zr–Ti–Nb–(Al)-concentrated BCC alloys have entered the discussion from a neighboring composition space. They are not TiAl intermetallics in the strict phase-constitution sense, but they address a closely related design problem: how to combine low density, high strength, environmental stability and manufacturing tolerance in alloys built from Ti-, Nb- and Al-compatible chemistries.

Seen against this background, the central question addressed here is how Nb–Ti–Al-related lightweight alloys can be designed to combine service stability with deformation and processing accessibility. The discussion therefore treats high-temperature stability, microstructural deformation paths, composition-space expansion and processing accessibility as linked variables that determine whether a lightweight alloy can be manufactured and used. This design-space broadening is schematically illustrated in Figure 1.

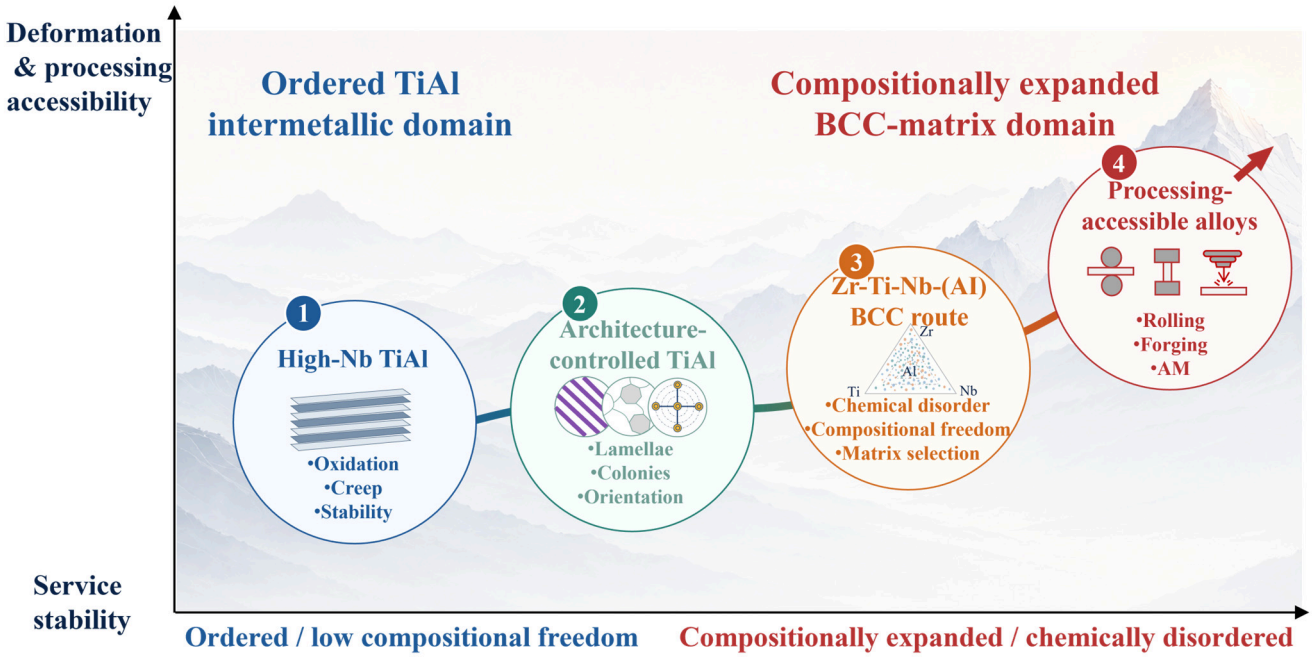



**Figure 1.** Design-space broadening in Nb–Ti–Al-related lightweight high-temperature alloys. The schematic connects the ordered TiAl intermetallic domain, where high-Nb TiAl first establishes service stability and architecture-controlled TiAl introduces lamellar/colony/orientation-mediated deformation paths, with the compositionally expanded BCC-matrix domain, where Zr–Ti–Nb–(Al) BCC routes and processing-accessible alloys shift deformability and manufacturability closer to the starting point of design. AM denotes additive manufacturing.

## 2. High-Nb TiAl and the Establishment of a Service-Stability Platform

The first major role of Nb in TiAl was to make the ordered intermetallic platform more credible for demanding environments. In high-Nb TiAl alloys, Nb strengthens the $\gamma/\alpha_2$ matrix, affects $\beta/B_2$ stability, and improves resistance to oxidation-related degrada-

tion [5]. These effects changed the design emphasis from merely producing a lightweight intermetallic to building a more durable high-temperature platform.

The service character of this route is evident in studies where environmental stability rather than tensile ductility is the primary metric. The following examples are used as illustrative cases, not as an exhaustive survey of TiAl environmental behavior. Laminated ceramic coatings on 8Nb-TiAl were developed to improve oxidation and spallation resistance at high temperature [6]. TiAl–Nb intermetallics were also examined in liquid-zinc corrosion environments, where corrosion life and surface condition became central concerns [7]. Such examples show that the significance of Nb-containing TiAl not only extends beyond strength, but also lies in extending the environmental and microstructural stability of an ordered low-density matrix.

This service platform, however, carries an intrinsic structural cost. The ordered $\gamma/\alpha_2$ framework is not a blank matrix to which ductility can simply be added. Deformation is filtered through crystallography, lamellar interfaces, and colony boundaries. As a result, high-Nb TiAl can be made stronger and more stable, but its manufacturability remains strongly dependent on how the ordered microstructure is arranged. This limitation led naturally to a second design emphasis: the deliberate construction of deformation pathways within the TiAl architecture.

## 3. Deformation Architecture Within Ordered TiAl Matrices

In TiAl alloys, plastic accommodation is controlled by architecture at several length scales. Lamellar spacing, colony size, $\beta/B_2$ distribution, grain orientation, and interface character determine whether dislocations and twins can carry strain without promoting cleavage [4]. The microstructure is more than a passive product of processing, as it acts as the medium facilitating deformation.

Several high-Nb TiAl studies illustrate this architectural emphasis. Gradient twin structures improved high-temperature tensile response by introducing a deformation substructure that interacts with the lamellar matrix [8]. Electron-beam melting showed that powder-bed processing can be applied to high-Nb TiAl when cracking, segregation and phase architecture are controlled [9]. TiC reinforcement, Si alloying and B addition refined colonies or modified second phases, thereby improving strength and damage tolerance through microstructural control [10–12]. Additively manufactured $\gamma$-based high-Nb TiAl composites further demonstrated that coherent interfaces and multiphase networks can suppress intergranular cracking and stabilize the microstructure during processing [13,14].

The polysynthetic-twinned Ti–45Al–8Nb single-crystal work remains a particularly clear example of architecture-controlled deformation. By regulating the beta-to-$\alpha$ transformation and lamellar orientation during directional solidification, favorable lamellar alignment was obtained without complex seeding. The resulting zero-degree-oriented specimens combined high room-temperature yield strength, measurable tensile ductility, and high strength with ductility at 900 °C [15]. The importance of this work lies not only in the numerical properties. It showed that a difficult deformation problem in TiAl can be approached through crystallographic architecture, variant selection and lamellar-interface design.

The ordered-matrix route therefore improves deformation primarily by engineering pathways through the $\gamma/\alpha_2$ framework rather than by removing the intrinsic restrictions of the ordered matrix. This insight becomes important when considering compositionally complex BCC alloys. If deformation in ordered TiAl must be recovered through architecture, an alternative is to begin from a matrix with broader intrinsic deformation capacity and then build strength and stability around it.

## 4. Compositionally Expanded Concentrated BCC Matrices as a Neighboring Design Route

Research on medium-/high-entropy alloys and multi-principal-element alloys introduced chemical disorder as an active design variable rather than a compositional complication [16–18]. This issue is particularly important for refractory BCC MPEAs, where high intrinsic strength is often accompanied by ductility and processing constraints [19]. Using the ideal expression $\Delta S_{conf}/R = -\Sigma\, x_i \ln x_i$, $Zr_{50}Ti_{35}Nb_{15}$ has an ideal configurational entropy of about 0.999$R$, while $(Zr_{0.5}Ti_{0.35}Nb_{0.15})_{97}Al_3$ and $(Zr_{0.5}Ti_{0.35}Nb_{0.15})_{80}Al_{20}$ have values of about 1.103$R$ and 1.299$R$, respectively. These values are below the conventional HEA threshold of 1.5$R$ and therefore support the use of MEA/MPEA terminology rather than classifying the alloys as HEAs on the basis of element number alone [17]. Within the Nb–Ti–Al-related lightweight-alloy landscape, the significance of Zr–Ti–Nb–(Al)-concentrated BCC matrices is that they approach the stability–deformability problem from the opposite direction: matrix deformability is considered at the beginning rather than recovered after an ordered matrix has been selected.

The $Zr_{50}Ti_{35}Nb_{15}$ alloy illustrates this change in starting point. Developed near the center of the Ti–Zr–Nb ternary phase diagram, it forms a single BCC solid solution and combines low Young's modulus with useful yield strength, tensile ductility, and corrosion resistance [20]. Its deformation involves dislocation slip and deformation twinning, indicating that concentrated BCC matrices can activate plasticity mechanisms that are difficult to use uniformly in ordered TiAl intermetallics.

Al addition adds a second design lever. In $(Zr_{0.5}Ti_{0.35}Nb_{0.15})_{100-x}Al_x$ alloys, nanoscale precipitates and diversified dislocation activity produced high strength while retaining useful ductility [21]. The broader implication is not simply that precipitation strengthening works in another alloy. Rather, chemical disorder provides a deformable BCC matrix, while Al can tune density, mixing enthalpy, precipitation tendency and potential environmental response. This sequence differs from the ordered-TiAl route because deformation compatibility is not treated only as a post-processing correction.

The size of the composition space makes efficient screening essential. Masking co-sputtering in Ti–Zr–Nb alloys allowed phase structure, modulus, hardness, and electrochemical behavior to be evaluated across many compositions [22]. Multi-target sputtering of Zr–Ti–Nb–Ta films further showed how phase stability and mechanical-property trends can be mapped in broader refractory composition spaces [23]. Surface modification of a Zr–Ti–Nb–Al alloy by micro-arc oxidation demonstrates one practical route for improving corrosion response, and also shows that environmental performance must be assessed together with BCC matrix design [24]. Recent work from other groups reinforces this broader view. Ti–Al–Nb–Zr and Ti–Zr–Nb–Al alloys show that Al content and Zr/Ti/Nb ratio affect BCC/$B_2$ stability, density and strength-ductility balance [25,26]. Ti–Zr–V–Nb–Al and Al–Ti–Zr–Nb–Ta lightweight refractory alloys further demonstrate the roles of grain refinement, $B_2$/BCC coherency and additive manufacturing in processing response [27,28]. Al-tuned Ti–Zr–Nb–Al refractory MEAs also show that Al/Nb adjustment can modify strength-ductility synergy in concentrated-BCC-related matrices [29]. These studies point to the same requirement: composition, valence electron concentration, density, oxygen affinity, phase stability and precipitation tendency must be evaluated as linked variables. Yet these variables become structurally meaningful only when they are connected to the mechanisms that accommodate deformation during processing. As summarized in Figure 2, the BCC route can therefore be viewed across three coupled length scales: atomic-scale chemical disorder, nanoscale Al-mediated phase regulation and mesoscale defect- and boundary-mediated deformation.

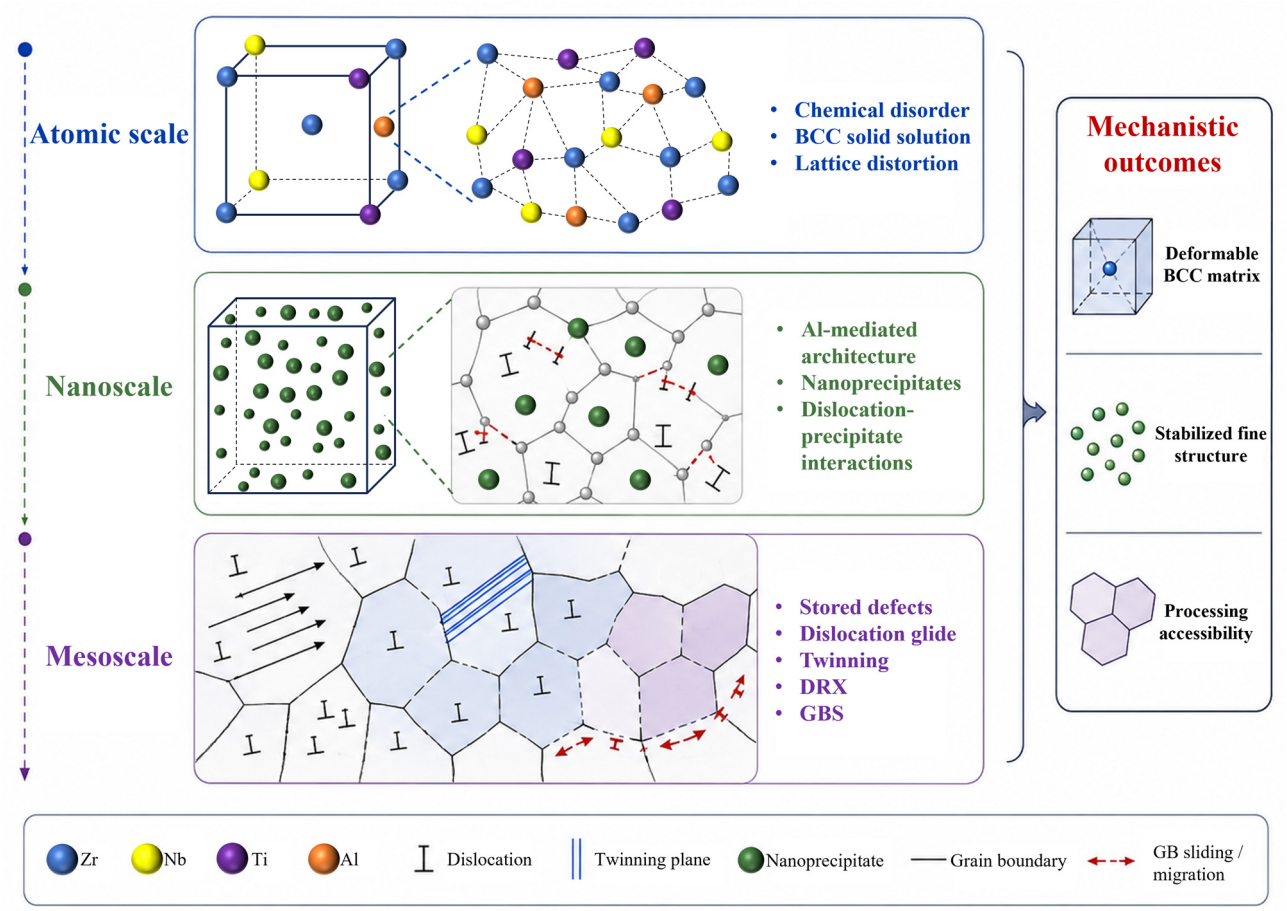



**Figure 2.** Multiscale bridge from chemical disorder to processing accommodation in Zr–Ti–Nb–(Al)-concentrated BCC matrices. Atomic-scale chemical disorder and BCC solid-solution formation provide a deformable matrix with local lattice distortion. Nanoscale Al-mediated phase architecture can regulate dislocation–precipitate interactions and fine-structure stability, while mesoscale stored defects, dislocation glide, twinning, dynamic recrystallization and grain-boundary sliding connect matrix deformability to processing accessibility.

## 5. Processing Accessibility and Designed Deformation Pathways

Building on this multiscale framework, intrinsic BCC matrix deformability is not sufficient by itself. For structural use, the alloy must convert that deformability into stable processing responses during rolling, forging, superplastic forming or other scalable shaping routes. Many BCC-concentrated alloys possess high strength but suffer from limited tensile ductility, dynamic recovery or strain localization. The Zr–Ti–Nb-based alloys are notable because they connect BCC chemical disorder with twinning, dislocation slip, dynamic recrystallization and grain-boundary sliding.

Cold-rolled $Zr_{50}Ti_{35}Nb_{15}$ provides a clear example. Pre-stored dislocations generated by rolling provide the driving force for dynamic recrystallization. Dynamic recrystallization and grain-boundary sliding alleviate local stress concentrations and achieve elongation reaching 200% under tensile deformation at 400–500 °C [30]. Prior deformation is therefore not merely a damage history. It becomes a stored-energy reservoir that can be used to activate subsequent plastic flow.

The Zr–Ti–Nb–Al superplasticity work extends this processing logic by adding nanoscale phase control. In $(Zr_{0.5}Ti_{0.35}Nb_{0.15})_{97}Al_3$, pre-stored dislocations promote dynamic recrystallization, while Al-induced nanoprecipitates hinder grain growth and stabilize the microstructure. A maximum elongation of 228% was achieved at 500 °C and a strain rate of $10^{-3}$ $s^{-1}$ [31]. This response is consistent with the broader understanding that

dynamic recrystallization depends on stored energy, recovery kinetics, temperature, strain rate, and grain-boundary evolution [32,33].

Precipitates therefore acquire a different role in a processability-centered BCC matrix. In classical strengthening, they are often judged mainly by their ability to impede dislocations. During high-temperature deformation, however, particles also affect grain growth, recrystallization stability, and the persistence of fine grains [34]. The useful precipitate population must be strong enough to stabilize a deforming microstructure but not so coarse or brittle that it becomes a crack-initiation source. Processing accessibility is thus a coupled outcome of matrix chemistry, defect storage, recrystallization kinetics and phase stability. Table 1 summarizes the route-level contrasts among these alloy systems and design strategies.

**Table 1.** Comparative summary of the alloy systems and design routes discussed in this Perspective.

| Design Route/ Representative Systems | Matrix or Phase Constitution | Main Design Focus | Representative Response or Property Emphasis | Remaining Limitation or Open Issue |
|---|---|---|---|---|
| High-Nb TiAl service platform; TiAl–Nb and 8Nb–TiAl examples [5–7] | Ordered $\gamma/\alpha_2$ TiAl matrix, with Nb affecting $\beta/B_2$ stability and environmental response | Improve high-temperature strength, oxidation resistance and creep/environmental stability | Nb strengthens the ordered matrix and improves service relevance; coating and corrosion examples illustrate environmental metrics | Room-temperature plasticity and workability remain limited by ordered bonding and lamellar anisotropy |
| Architecture-controlled high-Nb TiAl [8–15] | Lamellar/colony structures, twins, texture, $\beta/B_2$ distribution, coherent interfaces and PST-like orientation control | Recover deformation pathways within an ordered intermetallic framework | Gradient twins, refined colonies, reinforcement/alloying, additive manufacturing and PST single crystals improve strength-ductility or processing response | Benefits depend strongly on precise processing, texture/orientation control and interface stability |
| $Zr_{50}Ti_{35}Nb_{15}$-concentrated BCC/MEA route [20,30] | Single BCC solid solution; ideal configurational entropy $\approx 0.999R$ | Select a deformable BCC matrix before adding strengthening and stability variables | Low Young's modulus, useful strength/ductility and corrosion resistance; deformation by slip and twinning; near-superplastic response after cold rolling | Long-term high-temperature stability and component-scale validation remain to be established |
| Al-containing Zr–Ti–Nb–(Al) BCC matrices [21,24,31] | Concentrated BCC matrix with Al-mediated precipitates or surface/oxide modifications depending on composition and processing | Couple BCC matrix deformability with density control, precipitation and microstructural stabilization | Nanoprecipitates and stored dislocations can enable high strength, useful ductility and superplastic elongation; MAO coatings improve corrosion response | Phase stability, precipitate coarsening/brittleness and environmental durability require systematic validation |
| Recent related Ti/Zr/Nb/Al-based BCC MPEAs from other groups [25–29] | Single BCC, BCC/$B_2$ or metastable BCC-related matrices in Ti–Al–Nb–Zr, Ti–Zr–Nb–Al, Ti–Zr–V–Nb–Al and Al–Ti–Zr–Nb–Ta systems | Map Al/Zr/Ti/Nb/V/Ta effects on density, BCC/$B_2$ stability, grain refinement, dynamic response and additive manufacturability | Recent studies report high specific strength/ductility, grain-refinement-enabled uniform ductility, $B_2$/BCC strengthening and laser-directed energy-deposition feasibility | The broader design space increases the need for entropy/VEC/density/oxygen-affinity screening and bulk processing-service validation |

## 6. Outlook: Toward Processability–Stability Co-Design

The next stage of Nb–Ti–Al-related lightweight-alloy research is unlikely to be defined by a single new composition. The more important task is to connect design variables that have often been optimized separately. The first part of this Perspective has summarized literature-supported developments: TiAl research has established benchmarks for low density, oxidation resistance, creep resistance and microstructural stability, whereas concentrated BCC matrices provide a route to broader plastic accommodation and manufacturing tolerance. Against this background, the following discussion outlines prospective couplings that could move the field from separate optimization of composition, structure and processing toward processability–stability co-design. Neither route alone resolves the full problem of lightweight high-temperature structural materials.

One promising direction is the development of intermediate or duplex architectures that combine parts of the TiAl service advantage with the deformation tolerance of BCC chemical disorder. Such alloys would require careful control of $\beta/B_2$ stability, $\gamma/\alpha_2$ ordering, BCC solid-solution stability and precipitation reactions across processing and service

temperatures. Their value would not come from simply mixing two alloy concepts, but from using phase architecture to distribute deformation and stability functions between different structural units.

A second opportunity lies in defect and interstitial chemistry. Oxygen, nitrogen and carbon are often treated as impurities in high-temperature alloys, yet their interactions with Zr, Ti, Nb and Al can influence precipitation, ordering, grain-boundary cohesion and oxidation behavior. In Zr–Ti–Nb–(Al)-concentrated BCC matrices, controlled interstitial contents could become a design parameter, provided that their effects on ductility and environmental stability are quantified systematically.

A third requirement is to connect processing maps with service maps. Rolling, forging, additive manufacturing, and superplastic forming should be evaluated together with oxidation, creep, fatigue, and thermal cycling rather than treated as independent validation steps. In practice, efficient screening should combine CALPHAD or empirical parameters such as VEC and density, high-throughput experiments for phase/property mapping, bulk processing trials for scalability, and in situ or operando characterization to identify active deformation and degradation mechanisms. Curated property databases can then feed the next design cycle. Rather than seeking exhaustive control of every variable, the central goal is to establish a practical framework in which composition, phase architecture, deformation pathway and environmental stability are optimized together from the outset. These three couplings, hybrid phase architecture, defect/interstitial chemistry, and processing-service coupled maps, are summarized in Figure 3 as a route toward processability–stability co-design.

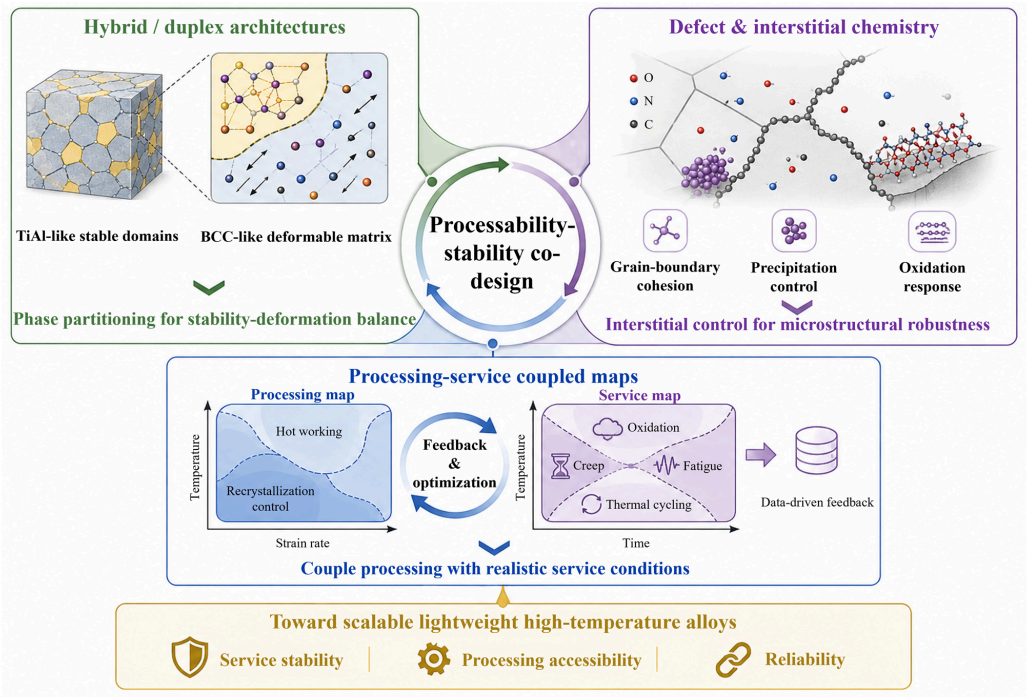



**Figure 3.** Outlook for processability–stability co-design in Nb–Ti–Al-related lightweight alloys. Three prospective couplings are highlighted: hybrid/duplex architectures that partition stability and deformation functions between TiAl-like stable domains and BCC-like deformable matrices; defect/interstitial chemistry linking O/N/C control to grain-boundary cohesion, precipitation and oxidation response; and processing-service coupled maps that integrate thermomechanical processing, realistic service conditions and data-driven feedback toward scalable lightweight high-temperature alloys. The arrows in the hybrid/duplex architecture denote atomic migration within the deformable BCC-like matrix.

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