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Hydrogen-based ore-to-part manufacturing of near-net-shape stainless steel

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Decarbonizing iron and steelmaking, combined with global disruptions to raw material supply chains, necessitates novel approaches to iron and steel production. In this work, we demonstrate a direct ore-to-part manufacturing route using a mixture of ore-derived oxide powders of Fe_2O_3 , Cr_2O_3 , NiO , and MoO_3 as feedstock for additive manufacturing, combined with sintering under H_2 to produce a near-net-shape austenitic stainless-steel. Complete reduction of all constituent oxides, including MoO_3 and Cr_2O_3 , is achieved in-situ at 1300 °C, resulting in dense, crack-free bulk alloy. The fabricated part retains geometric fidelity while undergoing substantial volumetric shrinkage inherent to redox and sintering. Thermodynamic calculations elucidate the co-reduction mechanisms and alloying pathways that enable complete metallization. This work is the first demonstration of net-shaping metal parts directly from ore derived oxides, and this ore-to-part approach can minimize the emissions and lead time for manufacturing associated with downstream processing such as rolling, forging, and machining.

The synthesis and processing of metals is the largest source of greenhouse gas emissions¹. Most metals occur in the Earth's crust as mixed oxides or sulfides, traditionally extracted via energy-intensive pyrometallurgical reduction using fossil-based agents (e.g., coke, coal), releasing CO_2 ¹. This approach is predominant for recovering transition metals such as iron, nickel, copper, chromium, cobalt, manganese, zinc, and tin from their oxidized forms². After extraction, additional processing is needed to produce application-ready parts, including liquid alloying, thermomechanical treatment (e.g., forging, rolling), machining, or shaping through extrusion or atomization followed by powder metallurgy or additive manufacturing. Thus, starting from extraction all the way to the final part production has their associated energy footprint thereby negatively impact economic sustainability.

H_2 -based redox reactions have emerged as a sustainable alternative to fossil reductant-based extraction, oxidizing H_2 to H_2O rather than CO_2 , directly supporting decarbonization³. Vacancy formation during H_2 redox promotes atomic interdiffusion, enabling solid-state alloying and mass transport for densification. Recent studies have demonstrated alloying from

mixed oxides (e.g., Fe-, Ni-, Cu-, Co-, Mo-, Cr-oxides), but under idealized conditions: nano-sized, high-purity powders shaped into micro-lattices and free from naturally occurring gangue oxides such as silicates (SiO_2) and alumina (Al_2O_3)⁴⁻⁶. In practice, gangue is inevitably present in industrial ores⁷; removing these gangues via separation or hydrometallurgy incurs substantial environmental costs. To realize the full potential of H_2 -based metallurgy at scale, two fundamental questions must be answered: (1) firstly, whether near-net-shape bulk components can be directly synthesized and (2) secondly, how trace gangue oxides influence alloying behavior and final microstructure. Resolving these questions is critical for advancing H_2 -based metallurgy toward industrial-scale, sustainable implementation.

To this end, we investigate a sustainable manufacturing paradigm: net-shaping of bulk alloy parts directly from mixed transition metal oxides through H_2 -based redox alloying, without extensive purification. This approach is demonstrated by manufacturing austenitic stainless steel one of the ubiquitous alloys with wide range of applications, while deliberately retaining realistic gangue levels. A suspension front bearing serves as a demonstrator to assess the feasibility of net-shaping. Furthermore, we

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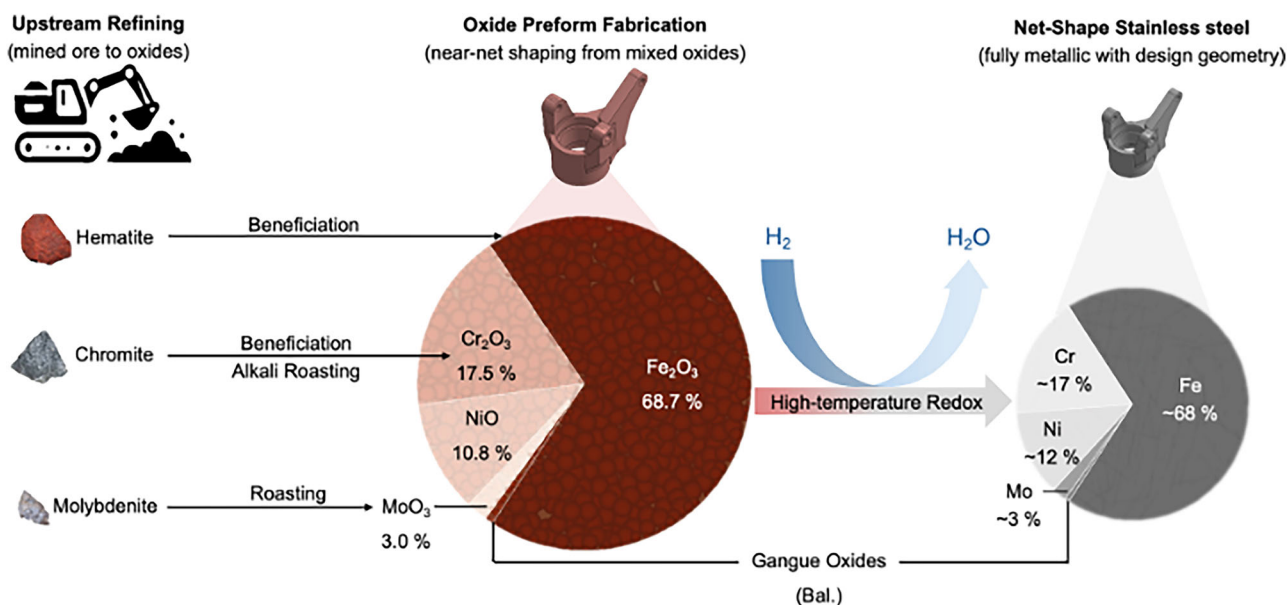
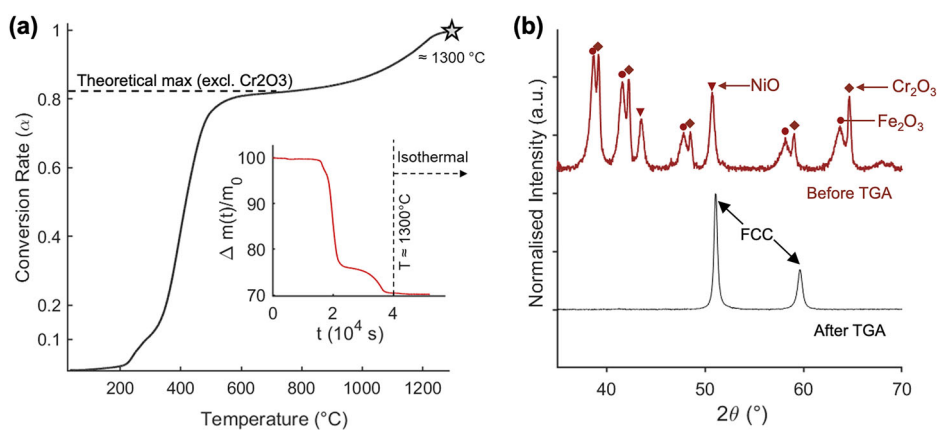


Fig. 1 | Conceptual schematic of ore-derived oxides to net-shape stainless steel via H_2 -based redox alloying.

Fig. 2 | Characterization of oxide mass and phase change upon H_2 -based redox. **a** Oxide-to-metal conversion (α) and instantaneous mass loss ($\Delta m(t)/m_0$) derived from TGA. **b** XRD patterns before and after TGA.



rationalize the sequential oxide reduction and alloying within mixed system using thermodynamic calculations, offering a new pathway for design oxide precursors as alloying agents.

Figure 1 outlines the proposed paradigm. The case-study alloy, austenitic stainless steel, comprises iron as the base matrix, with chromium for passivation and nickel and molybdenum for corrosion resistance. Iron and chromium are commonly derived from oxide-bearing mineral sources (e.g., hematite, chromite) that often coexists with alumina/silicate gangue partially removable via beneficiation (e.g., leaching, physical separation)⁸; alkali roasting may be used later for the subsequent extraction⁹. Molybdenum is commonly produced from molybdenite concentrates via oxidative roasting to molybdenum trioxide (MoO_3), which serves as the standard precursor to metallic Mo¹⁰. Nickel recovery is comparatively challenging because it only presented at low concentrations in lateritic or sulfidic ores¹¹. Although H_2 -based reduction of nickel sulfides is thermodynamically feasible, the presence of sulfur complicates processing¹²; therefore, nickel oxide (NiO) is used here as a simplified carrier to model nickel addition. Overall, the selected oxides serve as industrially relevant model feedstocks. These oxides are mixed and shaped into a preform with a geometry close to the final part. Upon exposure to H_2 and high-temperature, the preform undergoes redox-driven reactions form metallic stainless steel part. During this process, shrinkage driven by oxygen removal and porosity closure is expected; however, this dimensional change can be compensated for through design.

Results

Oxides-to-metal conversion

Among the transition metal oxides presented in the mixture (Supplementary Fig. S1), Fe_2O_3 , NiO , or MoO_3 are unstable phases under H_2 below 1300 °C^{13,14}, while reduction of Cr_2O_3 is only thermodynamically feasible under carbon-based reductant at 1300 °C, as widely utilized in ferrochromium production using CH_4 - H_2 mixtures¹⁵. Experimentally, the reducibility of the mixed oxides under H_2 was evaluated using a slow ramp of 1 K/min up to 1300 °C. The extent of oxides-to-metal conversion, defined as $\alpha = (\text{oxygen removed})/(\text{total oxygen initially present})$, was derived from TGA measurement and plotted in Fig. 2a. The α -curve climbs to $\alpha \approx 0.81$ by 700 °C, surpassing the theoretical maximum α if assuming Cr_2O_3 remains unreduced. The inset, which displays the instantaneous mass loss rate, highlights that most of the reduction occurred rapidly below 700 °C. Above this temperature, the reduction progresses asymptotically as α approach unity where all transition metal oxides were fully metalized when approaching 1300 °C. Ex-situ XRD patterns in Fig. 2b corroborate the complete reduction, including that of Cr_2O_3 , and reveal a transformation from mixed oxides phases to a single set of FCC reflections. This suggests that the reduced Fe, Ni, Cr, and Mo atoms have been successfully incorporated into a solid solution, forming an austenitic matrix. EDS analysis from four scan areas of 2500 μm^2 across the TGA sample cross-section showed an average composition of $Fe_{68.11 \pm 0.43} Cr_{16.74 \pm 0.34} Ni_{12.01 \pm 0.25}$

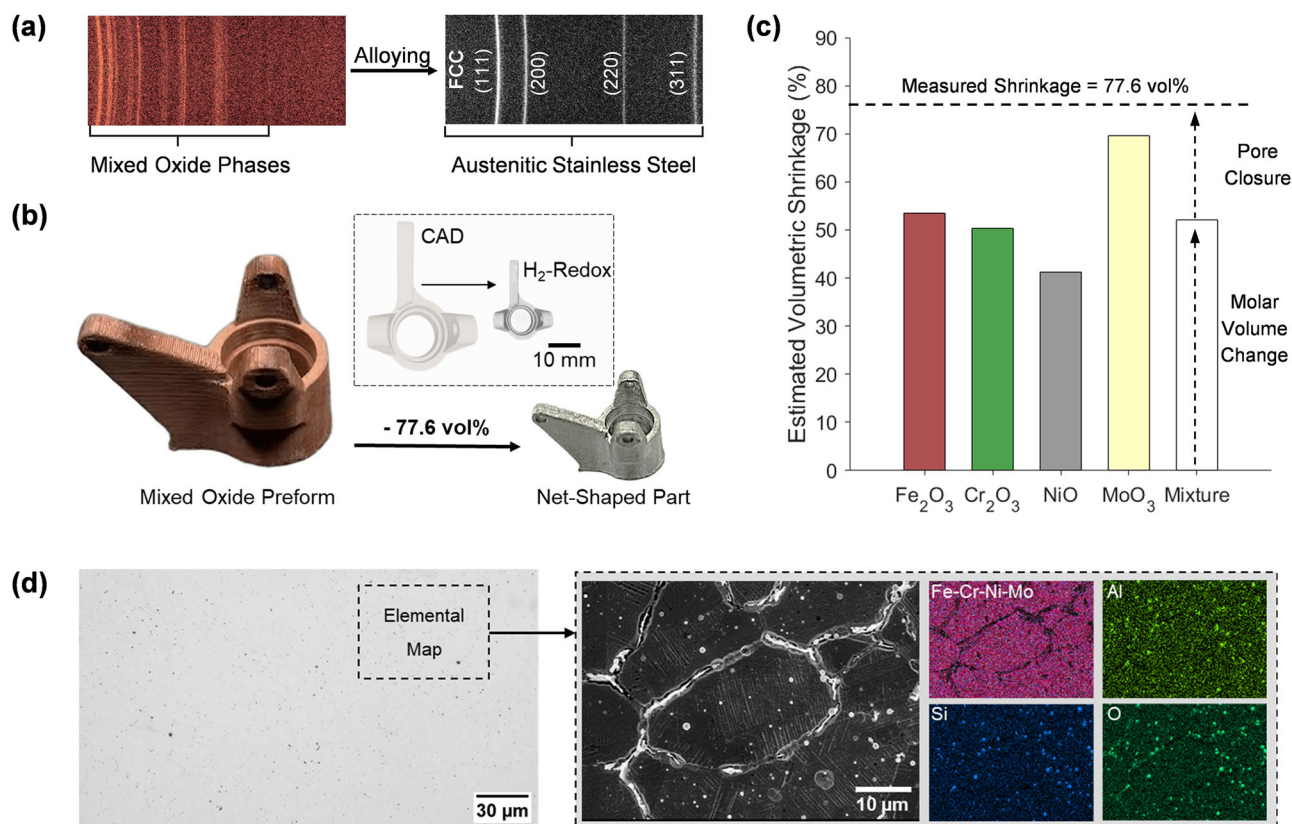


Fig. 3 | Macro- and microstructural evolution during H₂-based redox alloying. **a** X-ray diffractograms of the oxide mixture before and after H₂-based redox alloying in the tube furnace. **b** Photographs showing the geometrical changes of the gal-cast part.

c Comparison between theoretical shrinkage calculated from oxide reduction and the experimentally measured value. **d** Optical micrograph (left) and SEM-EDS maps (right) showing the dense microstructure decorated by Al- and Si-based particulates.

Mo_{2.34±0.61} (wt.%), confirming a near-complete reduction of all transition metal oxides to form the targeted Fe₆₈Cr₁₇Ni₁₂Mo₃.

Macro- and micro-structural evolution

The reducibility of the oxide mixture was further evaluated using gel-cast parts processed under a tube furnace with the same heating rate (1 K/min) as in the TGA experiment. X-ray diffractograms collected from the center of the sample cross-section reaffirmed a complete transformation to a single FCC phase following H₂-redox (Fig. 3a), accompanied by a distinct color change from hematite red to metallic silver (Fig. 3b). Dimensional comparison against the original CAD model revealed a substantial volumetric shrinkage of 77.6% (Fig. 3c), attributable to both redox-driven volume changes and sintering-induced densification. The theoretical shrinkage due to metalization of oxides can be approximated from the molar volume ratio of the pure metal (V_{metal}) and its oxide (V_{oxide}): $1 - nV_{metal}/V_{oxide}$, where n is the number of metal atoms per mole volume of oxide. Applying a composite theory (i.e., mass-weighted rule of mixtures) to the present oxide composition yields a calculated shrinkage of 52.4 vol.%, due solely to molar volume change during reduction (Fig. 3c). The remaining shrinkage is ascribed to the densification via pore closure. Notably, despite the high shrinkage observed, the final geometry exhibits isotropic shrinkage and retains the intended design.

Microstructural analysis (Fig. 3d) shows a fully-dense, crack-free matrix with grain-level uniform distribution of Fe, Cr, Ni, and Mo, as a result of H₂-redox alloying. However, submicron inclusions, further resolved by SEM-EDS after Kalling etching, were identified as residual Si- and Al-based gangue oxides located at boundary areas and pore interfaces. These oxides remain chemically distinct, forming no detectable compound with transition metals, as further confirmed by EDS analyses on unetched microstructure (Supplementary Materials, Figs. S2 and S3). Prior studies on H₂-reduced iron ores have linked the presence of Si/Al oxides to swelling and

cracking due to their more than one order of magnitude thermal expansion mismatch with FCC-iron^{16–18}. However, no such macroscopic defects are observed here. Nonetheless, the gangue oxides consistently coincide with residual pores or reside at interfaces, both indicative of mechanical degradation due to stress concentration and interfacial debonding. It seems that purification of oxides to remove gangue elements are imperative if relying on ore-derived feedstock for direct net-shape manufacturing of metal components.

Collectively, these findings establish the feasibility of direct ore-to-part fabrication using H₂-based redox alloying, producing bulk components without geometrical deformation. However, the complete recovery of each element, specifically, Cr and Mo from their oxides under the solid-state H₂ sintering condition reported here, is still not well understood. Previous studies have reported significant Cr recovery (up to ~50 wt.%) from chromite ores via H₂ plasma smelting reduction to produce ferrochrome as the stainless steel precursor^{19,20}. Such plasma-assisted processes, however, operate under non-equilibrium conditions that differ fundamentally from the thermally driven gas–solid reduction reactions relevant to the present process. To gain insight into the reduction sequence leading to the formation of the final austenitic stainless steel, thermodynamic calculations were therefore performed.

Discussion

Firstly, equilibrium phase evolution for the ore-derived oxide mixture in H₂ is presented in Fig. 4a. Under equilibrium at low temperature, Fe₃O₄, FeCr₂O₄, NiO, and MoO₂ are stable. It is interesting to note that, none of the starting oxides, i.e., Fe₂O₃, MoO₃, Cr₂O₃, are stable at low temperature in the presence of H₂, indicating reaction between oxides to form stable products. As temperature increases, the reduction proceeds sequentially, beginning with MoO₂ → Mo, followed by NiO → Ni, and finally Fe₃O₄ → FeO → Fe and Cr₂O₃ → Cr. Upon formation of elemental Fe in BCC phase, subsequent

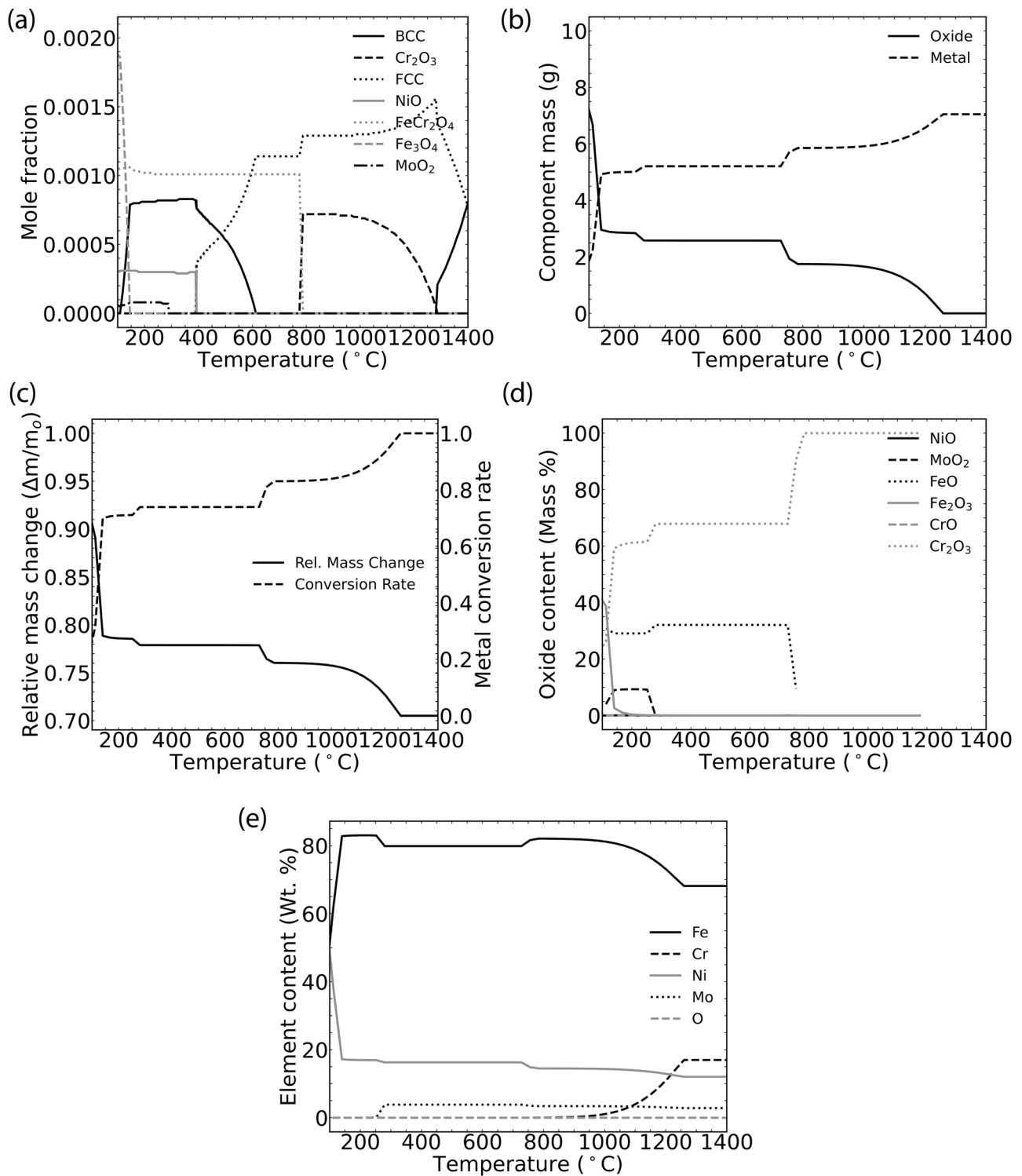


Fig. 4 | Thermodynamic and process metallurgy calculations of oxide reduction and metal formation during H₂-based redox alloying. a Equilibrium phase evolution for a mixture of oxide powders and excess H₂. b Process metallurgy calculation indicating amount of oxide and metal formed when considering 10 g of mixed

oxides in H₂. c Relative mass change and metal conversion rate corresponding to (b). d Evolution in constituents of oxides with reduction temperature. e Evolution of metal composition with reduction temperature.

reduction products like Ni, Mo, and Cr dissolve progressively into the BCC of Fe matrix, ultimately forming austenitic stainless steel (FCC phase in Fig. 4a). To quantify this reduction sequence under experimental conditions as shown in the TGA data in Fig. 2, thermodynamic calculations were performed based on the reduction of 10 g of ore derived oxide mixture using 100 g of H₂ (100 g was assumed to simulate the continuous flow of H₂).

Figure 4b shows the evolution of oxide and metal masses as a function of temperature. Initially, the system contains 10 g of oxide. As the temperature increases, the formation of metallic species begins, accompanied by a progressive reduction in oxide mass. Approaching 1250 °C, the metal mass reaches ~ 7 g, while the oxide mass is fully depleted. Beyond 1250 °C, the masses of both metal and oxide plateau, indicating that the completion of

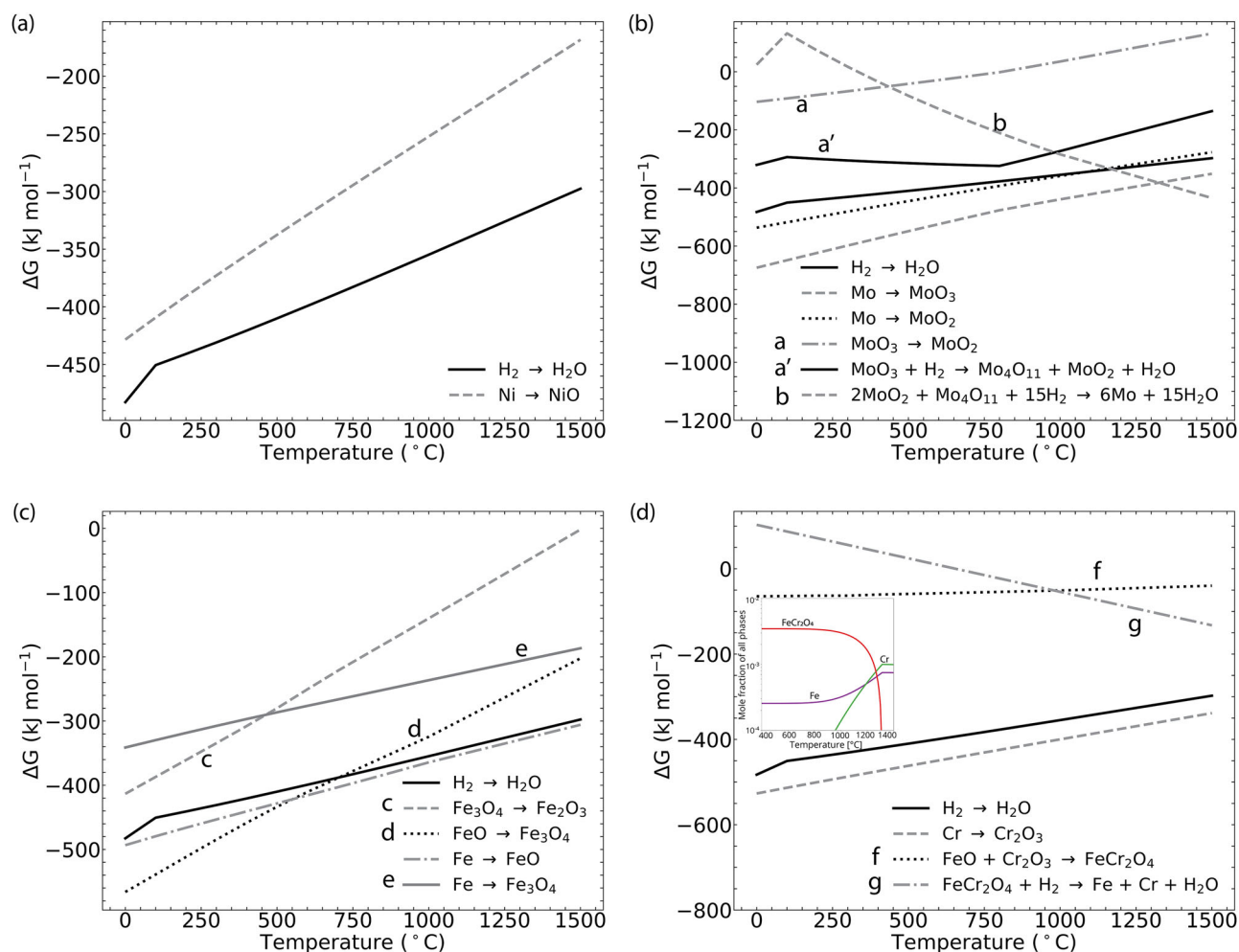


Fig. 5 | Gibbs free energy curves for reduction reactions. Curves showing reduction behaviour of: **a** NiO, **b** MoO₃, **c** Fe₂O₃, and **d** Cr₂O₃.

the reduction process. To validate the thermodynamic simulation against the TGA data presented in Fig. 2, the relative mass change and metals conversion were calculated and are plotted in Fig. 4c. The close agreement between the nature of the curve in Fig. 4c and the experimental TGA in Fig. 2b supports confidence in the thermodynamic calculations. To further resolve the reduction sequence and the composition of the metal obtained, the constituents of oxides and metal composition are shown in Fig. 4d, e, respectively. The results indicate that NiO readily reduces first, followed by MoO₂. The absence of MoO₃ in Fig. 4d suggests an immediate conversion to MoO₂. Subsequently, Fe₂O₃ reduces further into FeO, while both FeO and Cr₂O₃ gradually reduce as temperature increases. This stepwise reduction is directly reflected in the evolving metallic composition shown in Fig. 4e.

From the results presented in Fig. 4, it is clear that the reduction proceeds sequentially as NiO→Ni, MoO₃→Mo, Fe₂O₃→Fe, and finally Cr₂O₃→Cr. Going purely by the Ellingham diagram²¹, only the reduction of NiO→Ni by H₂ can be directly explained. The reduction mechanisms for the remaining oxides, necessitate further discussion.

Considering the sequential reduction of the four compounds, Fig. 5 demonstrates the thermodynamic spontaneity of their respective reduction steps. Figure 5a shows the Gibbs free energy curves for oxidation reactions of Ni and H₂. The diagram clearly indicates that NiO reduction by H₂ is thermodynamically favorable, elucidating why Ni is the first metallic species formed during the reduction (Ref. Fig. 4e).

Figure 4a, d indicate clearly that MoO₃ is not a stable oxide under these conditions; instead, MoO₂ is thermodynamically favored. As illustrated by the Gibbs free energy curves for Mo-based oxides in Fig. 5b, that the initial

reduction of MoO₃ to MoO₂ is highly favorable at low temperatures (Reaction a). This explains why MoO₂ is the dominant oxide phase at low temperatures, as observed in Fig. 4a, d. However, direct reduction of MoO₂ into Mo is thermodynamically unfavorable at low temperatures, suggesting an intermediate reduction step involving Mo₄O₁₁ (Reaction a' in Fig. 5b). Lalik²², using in situ neutron diffraction, have confirmed Mo₄O₁₁ as an intermediate oxide formed during MoO₃ reduction to MoO₂. Therefore, we propose that MoO₃ initially reduces to MoO₂ and Mo₄O₁₁ (Reaction a', Fig. 5b), and subsequently, the combined MoO₂ and Mo₄O₁₁ phases undergo further reduction to metallic Mo via Reaction b. The final reduction becomes thermodynamically feasible above 280–300 °C, corresponding precisely to the observed temperature at which Mo partitions into the metallic phase in Fig. 4e. Thus, the reduction of MoO₂ to metallic Mo occurs fully between 280 and 400 °C.

Fe₂O₃ readily reduces into magnetite (Fe₃O₄) under H₂, as illustrated by Reaction c in Fig. 5c. Near approximately 400 °C, the formed Fe₃O₄ is further reduced to metallic Fe (Reaction e, Fig. 5c), explaining the observed increase in Fe content in the metal phase. Furthermore, above 650–700 °C, any remaining Fe₃O₄ can further reduce to FeO (Reaction d, Fig. 5c), accounting for the presence of FeO observed in Fig. 4d.

Similar to MoO₂, Cr₂O₃ is challenging to reduce solely under H₂. However, several studies have reported the reduction of Cr₂O₃ under H₂ at relatively lower temperatures. For example, Radomysel'sii et al.²³ investigated the co-reduction of Fe₂O₃ and Cr₂O₃ under H₂ targeting Fe-20Cr (wt.%) composition. They observed only trace amount of Cr₂O₃ after 7 h at 1100 °C and speculated that the thermodynamic driving force

originating from reduced Fe_2O_3 facilitated the reduction of Cr_2O_3 . This observation underscores a critical limitation of the classical Ellingham diagram, which assumes that the activity of the metal α_{Me} as unity, thus it models oxidation of pure metals exclusively. In multicomponent alloy systems, where $\alpha_{Me} < 1$, the Gibbs free energy barrier for oxide reduction is effectively lowered. The equilibrium conditions for oxidation in such multicomponent systems are more accurately described by the modified relation²⁴:

$$RT \ln p_{\text{O}_2} = G^\circ - \frac{2a}{b} RT \ln \alpha_{Me} \quad (1)$$

where G° is the standard oxidation reaction of the pure metal, and a and b refer to the stoichiometry of the metal oxidation $\frac{2a}{b} \text{Me} + \text{O}_2 \rightarrow \frac{2}{b} \text{M}_{\text{e}a} \text{O}_b$. For instance, assuming an ideal $\text{Fe}_{68}\text{Cr}_{17}\text{Ni}_{12}\text{Mo}_3$ (wt.%) solution with $\alpha_{Me} \approx 0.18$, the driving force for Cr_2O_3 reduction (quantified by $G_{\text{oxide}}^\circ - G_{\text{H}_2\text{O}}^\circ$ value) shifts by ~ 39 kJ/mol toward spontaneity. Similarly, more recent study conducted by Shankar et al.²⁵ reported that in mixed oxide systems, the reduced activity of Cr in the metallic phase could aid in lowering the reduction temperature of Cr_2O_3 .

From the perspective of lowering thermodynamic barrier for such reaction, we propose an additional mechanism to explain the observed low temperature reduction of Cr_2O_3 . As previously discussed for Fe_2O_3 , residual Fe_3O_4 can undergo reduction into FeO beyond 600 °C (Reaction d, Fig. 5c), with the presence of FeO further supported by thermodynamic calculations in Fig. 4d. FeO and Cr_2O_3 can react to form spinel based FeCr_2O_4 via Reaction f in Fig. 5d, which is thermodynamically favorable, as indicated by the equilibrium calculations in Fig. 4a. The FeCr_2O_4 spinel can undergo reduction to metallic Fe and Cr via Reaction g in Fig. 5d. It should be noted that this reaction is thermodynamically feasible above ~ 1000 °C, corresponding to the temperature range where Cr partition into the metallic phase is observed. Furthermore, the inset in Fig. 5d confirms that the reduction of FeCr_2O_4 under H_2 becomes thermodynamically favorable above 1000 °C, with the complete reduction achieved close to 1280 °C.

In summary, we demonstrate that using ore derived oxides as feedstock for additive manufacturing, followed by sintering under H_2 atmosphere is a viable manufacturing route to transform extracted ore into near-net-shape parts. We demonstrate this concept using mixed oxide system comprising Fe_2O_3 , Cr_2O_3 , NiO, and MoO_3 to fabricate bulk near-net-shaped austenitic stainless steel part. Based on experimental and thermodynamic results, the following conclusions can be drawn:

- (i) H_2 -based redox directly transforms sustainable oxide preforms into net-shape bulk metal parts. Alloying and densification can proceed even in the presence of minor Al and Si-based gangue impurities; however, these impurities tend to reside within residual pores and at interfaces. Shrinkage during oxide metalization is significant but uniform, in contrast to classical powder sintering where differential shrinkage often leads to slumping and distortion.
- (ii) Phase transformations between oxides within the mixed system can alter the reduction pathway and lower the reduction temperature relative to pure single oxides, thereby assisting in the reduction of otherwise difficult-to-reduce under H_2 . We propose this mechanism as the main pathway for the reduction of MoO_3 and Cr_2O_3 during the formation of austenitic stainless steel.
- (iii) Complete reduction of difficult-to-reduce oxides by exploiting oxide-to-oxide phase transformation can open up new avenues in CO_2 -free steel production and on-the-fly alloying and can potentially provides a pathway to reduce refractory oxides (Nb, W, and V) with comparable stability under H_2 .

Together, these findings lay the foundation for utilization metallic ores as of sustainable, low-cost feedstocks for direct net-shape metal manufacturing.

Methods

Near-net-shape manufacturing of oxide mixture

For our investigation, micronized Fe_2O_3 (KREMER Pigmente, $D_{90} = 5.91$ μm), Cr_2O_3 (KREMER Pigmente, $D_{90} = 3.42$ μm), NiO (Alfa Aesar, 400 mesh), and MoO_3 (Sigma Aldrich, ~ 100 nm) powders were blended to a nominal composition of 316 grade austenitic stainless steel (17Cr–12Ni–3Mo–68Fe (wt.)) after complete oxide reduction (Fig. 1). The oxide mixture was homogenized via low-energy ball milling (250 rpm, 4 h, ball-to-powder ratio 10:1), then shaped into a suspension bearing using gel-casting following established protocols described in ref. 26. Gangue impurities were introduced through the Fe_2O_3 pigment, contributing 0.34 wt.% Si and 0.36 wt.% Al.

Oxide reduction experiments

Redox test of the oxide mixture (without binder) was performed using thermogravimetric analysis (TGA; STA 449F3, Netzsch). A sample mass of 107.41 mg was subjected to a flowing H_2 atmosphere (99.999% purity, Linde AG) at 100 mL/min. The thermal profile consists of heating at 1 °C/min to 1300 °C, followed by a 2 h of isothermal hold. The measurement was repeated under identical conditions. Redox test of gel-casted demonstrators was conducted in a tube furnace (Elektromat Dresden) under flowing H_2 at 2.5 L/min. A debinding step was first performed at 500 °C for 1 h, followed by redox processing using the same thermal profile as employed in the TGA experiments.

Macro- and micro-structural characterizations and analysis

Post-reduction geometries were measured using a contact-free optical scanner (ALCON, Hexagon) and compared with the original computer-aided design (CAD) model to quantify volumetric shrinkage (vol%) and evaluate geometrical distortion. Phase analysis of the ball-milled mixture and redox specimens were conducted via X-ray diffraction (XRD; D8 DISCOVER, Bruker) using a Cobalt source (Co-K α , $\lambda = 1.79026$ Å), operated at 40 kV and 45 mA. Microstructural analysis was carried out using a field emission scanning electron microscopy (FESEM; Leo 1530, Zeiss) equipped with an energy dispersive spectroscopy (EDS) detector. Thermodynamic calculations presented were performed using TCOX10 oxides database of ThermoCalc in conjunction with the Process Metallurgy module of ThermoCalc^{27,28}.

Data availability

The datasets generated and/or analyzed during the current study are available within the article. Any additional data apart from what is provided are available from the corresponding author on reasonable request.

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Author contributions

M.Y. (Conceptualization; Formal analysis; Lead; Investigation; Methodology; Visualization; Writing—original draft; Writing—review & editing). R. K. (Formal analysis; Investigation; Visualization; Writing—original draft). M. K. (Investigation; Supporting; Visualization; Writing—review & editing). M. V. (Funding acquisition; Project administration; Supervision; Writing—review & editing). All authors reviewed and approved the manuscript for submission.

Competing interests

The authors declare no competing interests.

Additional information

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