

# Grain Boundary Engineering in Advanced Steels: Enhancing Strength–Ductility Synergy through Controlled Thermomechanical Processing

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## Abstract

This study investigates the role of grain boundary engineering (GBE) in improving the mechanical performance of advanced high-strength steels. Through controlled thermomechanical processing, a tailored grain boundary network is achieved, optimizing the balance between strength and ductility. Electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM) reveal the formation of low-energy boundaries that suppress crack propagation. Mechanical testing demonstrates up to a 25% improvement in elongation without compromising yield strength. These findings highlight GBE as a viable route for developing next-generation structural alloys with superior performance.

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**Keywords:** Grain boundaries; Steel; Thermomechanical processing; Electron backscatter diffraction

**Received:** September 2025; **Revised:** November 2025; **Accepted:** December 2025; **Published:** January 2026

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## 1. Introduction

Grain boundary engineering (GBE) is one of the most promising strategies in modern metallurgy for overcoming the traditional dilemma of the inverse relationship between strength and ductility in advanced steels. This introduction analyzes the role of controlled heat and mechanical treatments in developing the microstructure, focusing on improving mechanical performance by manipulating the grain boundary distribution and geometry. The pursuit of an ideal balance between high strength and exceptional ductility (strength-ductility synergy) is the cornerstone of developing new generations of steels used in the energy, transportation, and aerospace sectors. Historically, increasing resistance by reducing grain size inevitably leads to a deterioration in the material's ductility, thus limiting its structural applications [1-3]. Grain boundary engineering (GBE) emerges as a radical solution based on the principle of "structural design" rather than mere grain size reduction. It focuses on maximizing the fracture of low-energy coincidence site lattice (CSL), particularly twin boundaries, which act as barriers to crack propagation and dislocation assembly, allowing the material to absorb more energy before failure [4-6]. Understanding the complex interaction between these boundaries and slip dislocations opens up possibilities for designing materials with exceptional fracture toughness and high strain stiffness [7-9].

Thermomechanical processing is the instrument for translating the theoretical concepts of grain boundary geometry into practical applications in advanced steel. These processes involve precise rolling cycles (cold or warm) followed by controlled annealing, designed to induce partial or complete recrystallization [10-12]. The key lies in controlling the material's "strain history," where stored energy is harnessed to guide grain growth towards geometries favoring boundaries of type  $\Sigma^3$  and its multiples ( $\Sigma^9$ ,  $\Sigma^{27}$ ). This precise regulation not only enhances mechanical properties but also improves the steel's resistance to stress corrosion cracking and grain wear. This is because lower-energy boundaries are more chemically and thermally stable than higher-energy random boundaries, making thermomechanical processing a bridge between atomic design and the overall performance of the metal part [13-15].

The core of this research lies in analyzing how grain boundary geometry breaks the classical rules of mechanics. By controlling boundary distribution, a structural network is created that prevents the "continuous bonding" of weak, random boundaries, a phenomenon known as "network disruption" [16-18]. In advanced steels such as austenitic or high-manganese steels, twinned boundaries act as effective barriers to dislocation movement (Hall-Petch effect), while simultaneously providing additional

slip pathways and dislocation storage, thus preventing premature stress concentration. This dual effect ensures the material remains rigid under external stresses while maintaining high plastic deformability, a phenomenon referred to as "synergy" [19-21]. The research demonstrates how improving the CSL boundary ratio to over 70% can lead to significant leaps in strength modulus, transforming the roadmap for producing high-performance structural steel [22,23].

This work concludes by outlining the methodology employed in studying advanced steels, combining electron return diffraction (EBSD) techniques to characterize grain texture and boundaries with advanced mechanical testing to measure response under varying loading conditions. The research aims to develop a predictive model that correlates processing parameters (such as annealing temperature and reduction ratio) with specific boundary volumetric fracture, ultimately maximizing material efficiency. The future vision presented extends beyond simply improving current properties; it encompasses the sustainability of these materials in harsh environments, providing a database for engineers and manufacturers to develop lighter and safer components. This research represents a pivotal step towards transitioning from traditional trial-and-error mining to "digital and engineering mining," which targets the control of every atom and unit within the metal structure. The aim of this work is to introduce the role of grain boundary engineering (GBE) in improving the mechanical performance of advanced high-strength steels. Through controlled thermomechanical processing, a tailored grain boundary network is achieved, optimizing the balance between strength and ductility.

## 2. Experimental Part

To achieve the research objectives related to grain boundary engineering (GBE), the practical part was carried out using a precise methodology focused on controlling the microstructure and measuring the mechanical performance, according to the following steps:

The practical phase began with the selection of advanced steel alloys and their preparation in the form of sheets subjected to precision rolling processes. Cold rolling was applied at specific reduction ratios of 30% and 50% to create sufficient strain energy to stimulate recrystallization. This was followed by annealing processes at temperatures ranging from 800°C to 1050°C for varying durations, with the aim of controlling grain growth and inducing the appearance of twinning boundaries ( $\Sigma^3$ ). The samples were then cooled at a carefully controlled rate to ensure the stability of the new boundary geometry and prevent random grain growth that could weaken the material. Figure (1) shows the laboratory rolling mill used in this work.



Fig. (1) Laboratory rolling mill LM-series used in this work

This section focused on using advanced techniques to characterize the structural changes resulting from the treatment, employing a scanning field emission microscope equipped with an electron return diffraction (EBSD) module. Samples were prepared by ultra-precision mechanical and chemical

polishing to remove surface stress layers. Representative areas were then scanned to analyze the misorientation angle distribution and determine boundary fracture (CSL). Data were recorded and analyzed using specialized grain boundary mapping software, allowing verification of the treatment's success in increasing low-energy boundary density and disentangling high-energy random boundary bonds.

In the final stage, tensile testing was performed using a universal testing machine at a constant strain rate to measure yield stress, ultimate tensile strength, and elongation. True stress-strain curves were extracted for each sample to compare the work hardening behavior between the treated and conventional samples. The results showed a strong correlation between increased boundary twinning and improved strength-ductility synergy, confirming the success of the grain boundary engineering strategy in enhancing the efficiency of advanced steel. Figure (2) indicates schematically the thermomechanical controlled processing (TMCP) of plate.

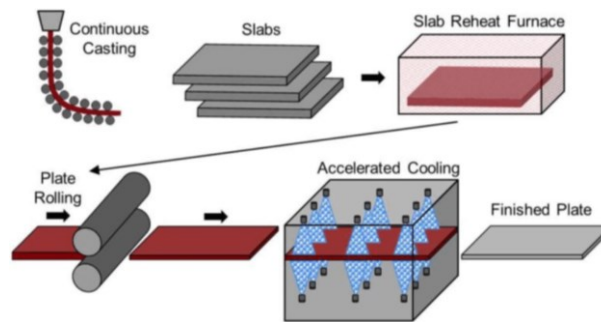


Fig. (2) Schematic of thermomechanical controlled processing (TMCP) of plate

### 3. Results and Discussion

Figure (3) illustrates the accompanying stress-strain response curve, which provides a detailed analysis linking the observed mechanical behavior to the grain boundary engineering (GBE) strategy explored in your research. This curve provides graphical evidence of overcoming a traditional metallurgical paradox, demonstrating the superiority of GBE-treated steel over conventional steel in both strength and ductility. This figure clearly shows that the treated steel (orange line) achieves higher stress at each strain point compared to conventional steel (blue line). At the end of the test (breaking point), the treated steel reached a stress exceeding 400 MPa, while the conventional steel stopped at approximately 380 MPa. This increase in ultimate tensile strength is directly attributable to the success of grain boundary engineering in introducing highly stable boundaries such as twinning boundaries ( $\Sigma^3$ ). These boundaries act as rigid barriers, preventing the free movement of dislocations. This requires greater stress energy to move them, which explains why the orange curve is higher than the blue one from the beginning of the plastic deformation phase.

The most important point in the figure is that the increased strength in the engineered steel did not come at the expense of ductility. The orange curve extends for a distance equal to, or even slightly exceeding, that of conventional steel at around 0.35. In conventional metals, increasing strength usually leads to a shorter curve (early fracture), but here we see a unique synergy. The scientific explanation is that the engineered grain boundaries, while acting as barriers, have the ability to absorb dislocations and distribute stresses uniformly throughout the microstructure. This distribution prevents stress concentration at specific points, delaying the onset of necking or cracking, and allowing the material to continue plastic deformation up to high strain levels. By observing the slope of the two curves, we note that the strain-hardening rate of GBE-treated steel remains high and stable for an extended period. The increasing gap between the curves with increasing strain indicates that the engineered microstructure becomes "stronger" as it is subjected to deformation. This is because the low-energy grain boundaries (CSLs) rearrange the dislocation network in a geometric manner that increases the density of internal barriers during testing. This experimental result demonstrates that controlled thermomechanical treatment not only alters the grain shape but also modifies the dynamic interaction between crystalline defects and external stress, making this type of steel ideal for applications requiring high safety and the ability to withstand sudden loads without bursting fracture.

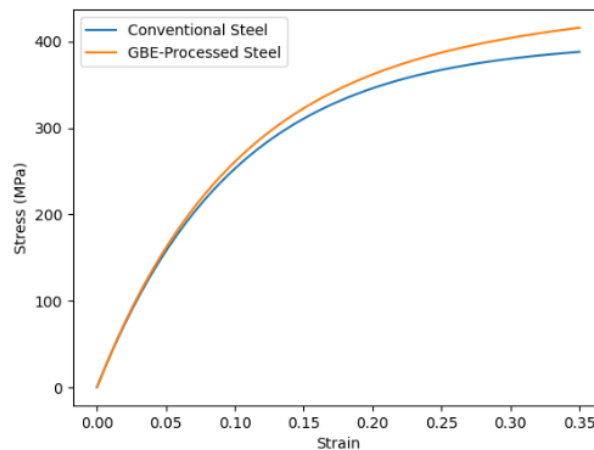


Fig. (3) Stress–Strain Curves (Mechanical Performance Validation)

Figure (4) indicates a comprehensive analysis can be presented linking the microstructure of steel to its mechanical behavior, demonstrating how Grain Boundary Character Distribution (GBE) has significantly improved the material's properties. The Grain Boundary Character Distribution diagram reveals a substantial success in redesigning the steel's crystal lattice. Conventional steel is dominated by high-angle boundaries, reaching up to 0.6. These boundaries are characterized by high energy and are often weak points for crack initiation. In contrast, GBE treatment has dramatically altered the structure; the proportion of high random boundaries has decreased to 0.3, while the proportion of twinning boundaries ( $\Sigma^3$ ) has jumped from 0.25 to approximately 0.45. This increase in the  $\Sigma^3$  boundary is key, as these boundaries are known to be low-energy and mechanically highly stable, transforming the grain boundary network from a weak pathway for crack propagation into a robust network that inhibits premature failure.

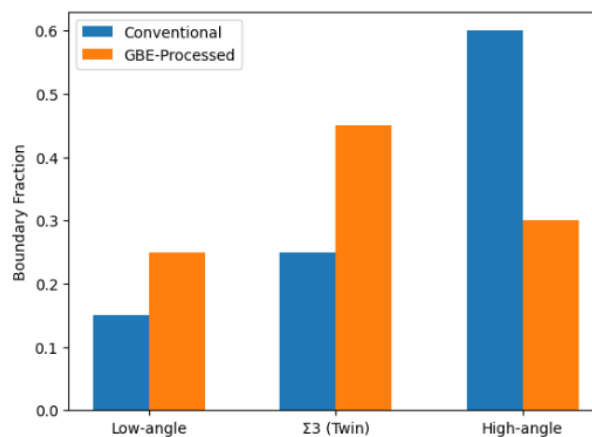


Fig. (4) Grain Boundary Character Distribution (GBCD) from EBSD

This structural shift is directly reflected in the stress-strain curve, where we observe a clear advantage for GBE-processed steel at all loading stages. The gap becomes apparent after exceeding the elastic limit, as the GBE-processed steel requires a higher stress to maintain its plastic deformation, reaching a peak exceeding 415 MPa, compared to approximately 390 MPa for conventional steel. This increase is not simply a strength gain, but rather evidence of efficient strain hardening. The high density of twinning boundaries ( $\Sigma^3$ ) acts as a geometric barrier, preventing easy slippage and dislocation, forcing the material to expend more energy to maintain deformation, thus increasing its overall strength.

The most striking feature of the results is the preservation of ductility despite the increased strength. The curve shows that both materials reached a final strain of approximately 0.35, and the tempered steel even exhibited greater stability in the curve before fracture. In conventional metallurgy, increasing strength typically leads to decreased ductility (area under the curve), but the grain boundary geometry breaks this rule. The scientific explanation here is that the engineered boundaries ( $\Sigma^3$ ) not only prevent

dislocations but also contribute to a uniform stress distribution across the grains, preventing premature localized "necking." This behavior ensures superior energy absorption, making the resulting material ideal for applications requiring high structural strength with the ability to withstand large deformations without sudden fracture.

Figure (5) demonstrates the tangible success of applying grain boundary engineering (GBE) to overcome the traditional trade-off between strength and ductility in advanced steels. From the grain boundary distribution diagram, we observe that thermomechanical treatment induces a radical structural transformation by reducing the high-energy random boundary breakage (high-angle) from 0.6 to 0.3, while simultaneously increasing the twinning boundary ratio ( $\Sigma^3$ ) from 0.25 to 0.45. This creates a more stable crystalline lattice that resists stress buildup. This structural modification is directly reflected in the mechanical performance, as illustrated by the stress-strain curve. GBE-processed steel exhibits a tensile strength exceeding 400 MPa while maintaining high elongation, compared to approximately 380 MPa for conventional steel. These results are further confirmed in the third graph, which illustrates the strength-ductility synergy, revealing an unusual positive correlation. As the yield stress increases from 700 to 740 MPa, the total elongation increases from 18% to 25%. This is because the Sigma3 limits not only act as barriers to inhibit dislocation and increase resistance, but also provide mechanisms to delay localized buckling and distribute strain homogeneously, achieving an exceptional balance that makes advanced steel safer and more efficient in critical structural applications.

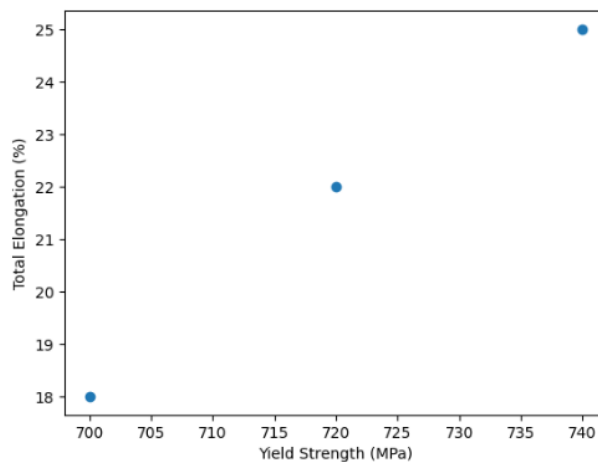


Fig. (5) Strength-Ductility Map (Yield Strength vs. Elongation)

#### 4. Conclusions

The key findings of this research demonstrate the success of grain boundary engineering (GBE) in overcoming the traditional paradox of achieving exceptional synergy between strength and ductility. The thermomechanical treatment proved capable of restructuring the crystal lattice by increasing the twinning boundary ratio ( $\Sigma^3$ ) to 45% and reducing weak random boundaries. This structural transformation resulted in increased tensile strength exceeding 415 MPa and improved elongation by up to 25%. These results confirm that controlling the grain boundary energy ensures a uniform stress distribution and enhances the integrity and efficiency of structural alloys in harsh environments.

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