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Editorial

Microstructure and Properties in Metals and Alloys (Volume 2)

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1. Introduction and Scope

Microstructure design is key in targeting the desired material's properties. It is therefore essential to understand the relationship between these properties and the microstructure [1–10] and how to enhance them via a specific process [11–20], including, as an example, additive techniques. The following five journals participated in the current Topic: *Coatings*, *Alloys*, *Crystals*, *Materials*, and *Metals*. Contributions related to microstructure design and characterization were brought together as part of this Topic, combined with their association with the mechanical, fatigue, wear, and corrosion resistance of different types of metals and alloys. The goal of this Topic is to present contributions related to the relationship between the microstructure and properties of metals and alloys for different applications, including aeronautical and aerospace applications. Different process routes were considered (including thermo-mechanical routes and additive manufacturing) as a part of this Topic. Welding is a key issue in many applications; this is the reasoning as to why contributions related to welding are also included in this Topic.

2. Overview of the Published Articles

The present Topic includes nineteen research papers, one communication, and two review papers. Among the publications included, eleven papers were published in *Metals*, eight papers were published in *Materials*, two were published in *Crystals*, and one paper was published in *Coatings*, covering numerous aspects concerning microstructure–property relationships in the field of metals and alloys.

The contributions to the aforementioned journals are listed below:

1. Li, J.; Hu, B.; Zhao, L; Li, F.; He, J.; Wang, Q.; Liu, R. Influence of Heat Input on the microstructure and Impact Toughness in Weld Metal by High-Efficiency Submerged Arc Welding. *Metals* **2023**, *13*, 1217. https://doi.org/10.3390/met13071217.
2. Zuo, Z.; Hu. R.; Luo, X.; Tang, H.; Zhu, Z.; Gao, Z.; Li, J.; Zou, H.; Li. A.; Zhao, X.; Lai, Y., Li. S. Evolution Behavior of Rapidly Solidified Microstructure of a Ti-48Al-3Nb-1.5Ta Alloy Powder during Hot Isostatic Pressing. *Metals* **2023**, *13*, 1243. https://doi.org/10.3390/met13071243.
3. Xu, R.; Li, Y.; Yu, H. Microstructure Evolution and Dislocation Mechanism of a Third-Generation Single-Crystal Ni-Based Superalloy during Creep at 1170 °C. *Materials* **2023**, *16*, 5166. https://doi.org/10.3390/ma16145166.
4. Belov, N.; Akopyan, T.; Tsydenov, K.; Letyagin, N.; Fortuna, A. Structure Evolution and Mechanical Properties of Sheet Al–2Cu–1.5Mn–1Mg–1Zn (wt.%) Alloy Designed for $Al_{20}Cu_2Mn_3$ Disperoids. *Metals* **2023**, *13*, 1442. https://doi.org/10.3390/met13081442.
5. Rodriguez-Vargas, B.R.; Stornelli, G.; Folgarait, P.; Ridolfi, M.; Perez, A.F.M.; Di Schino, A. Recent Advances in Additive Manufacturing of Soft Magnetic Materials: A Review. *Materials* **2023**, *16*, 5610. https://doi.org/10.3390/ma16165610.

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6. Zhao, Q.; Qiao, Z.; Dong, J. Effect of Tempering Time on Carbide Evolution and Mechanical Properties of a Nb-V-Ti Micro-Alloyed Steel. *Metals* **2023**, *13*, 1495. https://doi.org/10.3390/met13081495.
7. Tan, D.; Fu, B.; Guan, W.; Li. Y.; Guo, Y.; Wei, L.; Ding, Y. Hierarchical Multiple Precursors Induced Heterogeneous Structures in Super Austenitic Stainless Steels by Cryogenic Rolling and Annealing. *Materials* **2023**, *16*, 6298. https://doi.org/10.3390/ma16186298.
8. Efzan, M.N.E.; Kong, J.K. The Properties and Microstructure of Na_2CO_3 and Al-10Sr Alloy Hybrid Modified LM6 Using Ladle Metallurgy Method. *Materials* **2023**, *16*, 6780. https://doi.org/10.3390/ma16206780.
9. Liu, G.; Jiao, M.; Yang, B.; Wang, Q.; Wang, J. A Phase Field Study of the Influence of External Loading on the Dynamics of Martensitic Phase Transformation. *Materials* **2023**, *16*, 6849. https://doi.org/10.3390/ma16216849.
10. He, B.; Wang, J.; Xu, W. Constitutive Models for the Strain Strengthening of Austenitic Stainless Steels at Cryogenic Temperatures with a Literature Review. *Metals* **2023**, *13*, 1894. https://doi.org/10.3390/met13111894.
11. Chu, D.J., Park, C.; Lee, J.; Jung, W.S. Effect of Ti/Al Ratio on Precipitation Behavior during Aging of Ni-Cr-Co-Based Superalloys. *Metals* **2023**, *13*, 1959. https://doi.org/10.3390/met13121959
12. Wang, Y.; Qin, X.; Lv, N.; Gao, L.; Sun, C.; Tong, Z.; Li, D. Microstructure Optimization for Design of Porous Tantalum Scaffolds Based on Mechanical Properties and Permeability. *Materials* **2023**, *16*, 7568. https://doi.org/10.3390/ma16247568.
13. Hernandez-Flores J.E., Rodriguez-Vargas, B.R.; Stornelli, G.; Perez, A.F.M.; Gaircia-Vazquez, F.d.J.; Gomez-Casas, J.; Di Schino, A. Evaluation of Austenitic Stainless Steel ER308 Coating on H13 Tool Steel by Robotic GMAW Process. *Metals* **2024**, *14*, 43. https://doi.org/10.3390/met14010043.
14. Lee, S.; Chokradjaroen, C.; Sawada, Y.; Yoon, S.; Saito, N. Regulated Phase Separation in Al–Ti–Cu–Co Alloys through Spark Plasma Sintering Process. *Materials* **2024**, *17*, 304. https://doi.org/10.3390/ma17020304.
15. Klančnik, G.; Burja, J.; Klančnik, U.; Šetina, B.; Krajinc, L.; Resnik, A. Microstructure and Properties variation of high-performance grey cast iron via small boron additions. *Crystals* **2024**, *14*, 103. https://doi.org/10.339/cryst14010103.
16. Wang, X.; Gao, X.; Jin, Y.; Zhang, Z.; Lai, Z.; Zhang, H.; Li, Y. Molecular Dynamics Simulation research on Fe atom precipitation behavior of Cu-Fe Alloys during the rapid solidification processes. *Materials* **2024**, *17*, 719. https://doi.org/10.3390/ma17030719.
17. Yang, L.; Zhang, H.; Zhao, X.; Lui, B.; Chen, X.; Zhou, L. Study on the microscopic mechanism of grain refinement of Al-Ti-B master alloy. *Metals* **2024**, *14*, 197. https://doi.org/10.3390/met1402019.
18. Li, X.; Wang, K.; Li, Y.; Wang, Z.; Zhao, Y.; Zhu, J. Mechanical and magnetic properties of porous $Ni_{50}Mn_{28}Ga_{22}$ shape memory alloy. *Metals* **2024**, *14*, 291. https://doi.org/10.3390/met14030291.
19. Morettini, G.; Landi, L.; Burattini, L.; Stornelli, G.; Foffi, G.; Di Schino, A.; Cianetti, F.; Braccesi, C. Application of the Theory of Critical Distance (TCD) to the Breakage of Cardboard Cutting Blades in Al7075 alloy. *Metals* **2024**, *14*, 301. https://doi.org/10.3390/met14030301.
20. R. Dong; J. Li; Z. Chen; W. Zhang; X. Zhou. Efect of deformation degree on microstructure and properties of nickel base alloys for forgings. *Metals* **2024**, *14*, 340. https://doi.org/10.3390/met14030340.
21. Sun, H.; Li, J.; Du, X; Xu, F.; Yan, S.; Li, X.; Li, Z.; Liu, B.; Pu, G. Improved high temperature stability and hydrogen penetration through a Pd/Ti composite membrane with TaTiNbZr intermediate layer. *Coatings* **2024**, *14*, 370. https://doi.org/10.390/coatings14030370.

22. Bajtosova, L.; Kihoulou, B.; Kralol, R.; H., J.; Cieslar, M. Nickel nanoparticles: insights into sintering dynamics. *Crystals* **2024**, *14*, 321. https://doi.org/10.390/crust14040321.

J. Li et al. (Contribution 1) report on the influence of heat input on the microstructure and impact toughness of weld metal via high-efficiency submerged arc welding. In their paper, weld metal was obtained through the process of welding at three different high heat inputs with laboratory-developed high-efficiency submerged arc welding wire for bridges. The effect of changing different high heat inputs on the microstructure and impact toughness of high-efficiency submerged arc weld metal was systematically investigated via cutting and Charpy V-notch impact tests at −40 °C through the use of optical microscopy, scanning electron microscopy, energy-dispersive electron spectroscopy, electron backscatter diffraction, and transmission electron microscopy for characterization and analysis. With the increase in heat input from 50 kJ/cm to 100 kJ/cm, the impact absorption energy decreased significantly from 130 J to 38 J. The number of inclusions in the weld metal significantly decreased and the size increased, which led to a significant decrease in the number of inclusions, thus effectively promoting acicular ferrite nucleation, further leading to a decrease in the proportion of acicular ferrite in the weld metal. Concurrently, the microstructure of the weld metal was significantly coarsened, the percentage of high-angle grain boundaries decreased, and the size of martensite/austenite constituents was significantly increased monotonically. The crack initiation energy was reduced by the coarsened martensite/austenite constituents and inclusions, which produced larger local stress concentrations, and the process of crack propagation took place with greater ease due to the coarsened microstructure and lower critical stress for crack instability propagation. The martensite/austenite constituents and inclusions in large sizes worked together to cause premature cleavage fracture of the impact specimen, which significantly deteriorated the impact toughness. The findings of this study showed that heat input should not exceed 75 kJ/cm for high-efficiency submerged arc welding wires for bridges.

Zuo et al. (Contribution 2) report on Ti-48Al-3Nb-1.5Ta powders manufactured from cast bars via the supreme-speed plasma rotating electrode process (SS-PREP) and used to prepare hot isostatically pressed (HIPed) material at 1050–1260 °C with 150 MPa for 4 h. The phase, microstructure, and mechanical performance were analyzed through the use of XRD and SEM, an electrical universal material testing machine, and other methods. The results showed that the phase constitution changed from γ phase to $\alpha 2$ phase and then to γ phase with the material changing from as-cast to powders and then to as-HIPed. Compared with the as-cast material, the grain size and element segregation were significantly reduced for both powders and as-HIPed. When the hot isostatic pressing (HIP) temperature was low, the genetic characteristics of the powder microstructure were evident. With the increase in the HIP temperature, the homogeneity of the composition and microstructure increased, and the prior particle boundaries (PPBs) gradually disappeared. The elastic moduli of the powder and as-HIPed were superior to those of th eas-cast, which increased with the increase in the HIP temperature. The hardness of as-HIPed was lower than that of the powder. The compressive strength, compressive strain, bending strength, and tensile strength of as-HIPed were higher than those of the as-cast. With the increase in the HIP temperature, the compressive strength decreased gradually, and the compressive strain was found to first decrease and then increase.

Xu et al. (Contribution 3) investigated the creep behavior and deformation mechanism of a third-generation single-crystal Ni-based superalloy at 1170 °C under a range of stress levels. Scanning electron microscopes (SEMs) and transmission electron microscopes (TEMs) were employed to observe the formation of a rafted γ' phase, which exhibits a topologically close-packed (TCP) structure. The orientation relationship and elemental composition of the TCP phase and matrix were analyzed to discern their impact on the creep properties of the alloy. The primary deformation mechanism of the examined alloy was identified as dislocation slipping within the γ matrix, accompanied by the climbing of dislocations over the rafted γ' phase during the initial stage of creep. In the later stages of creep, super-dislocations with Burgers vectors of a<010> and a/2<110> were observed

to shear into the γ' phase, originating from interfacial dislocation networks. Up to the fracture, the sequential activation of dislocation shearing in the primary and secondary slipping systems of the γ' phase occurs. As a consequence of this alternating dislocation shearing, a twist deformation of the rafted γ' phase ensued, ultimately contributing to the fracture mechanism observed in the alloy during creep.

Belov et al. (Contribution 4) studied the possibility of increasing the strength of non-heat-treatable sheet alloy Al2Cu1.5Mn (wt.%) through the joint addition of 1% Mg and 1% Zn. The effect of these elements on the structure and mechanical properties of the new sheet Al2Cu1.5Mn alloy designed for Al20Cu2Mn3 dispersoids was examined through calculations and the use of experimental methods. The obtained data on the phase composition, microstructure, and physical and mechanical properties of the new alloy for different processing routes (including hot rolling, cold rolling, and annealing) were compared with those for the ternary Mg- and Zn-free alloy. The authors showed that the formation of nanosized Al20Cu2Mn3 dispersoids (~7 vol.%) aids in the preservation of the non-recrystallized grain structure after annealing at up to 400 °C (3 h), while Mg and Zn have a positive effect on the strength due to the formation of alloyed aluminum solid solution. As a result, cold-rolled sheets of the Al2Cu1.5Mn1Mg1Zn model alloy showed substantially higher strength performance after annealing at 400 °C in comparison with the ternary reference alloy. Of note, the UTS was found to be ~360 vs. ~300 MPa and the YS was found to be 280 vs. 230 MPa. Regarding the Al2Cu1.5Mn1Mg1Zn model alloy, researchers have demonstrated that the system shows promise for the design of new heat-resistant alloys as a sustainable alternative to 2xxx alloys. This new alloy has an advantage over commercial alloys (particularly 2219, 2024, and 2014) not only in terms of manufacturability but also thermal stability. The sheet production cycle for the model alloy is much shorter because the stages of homogenization, solution treatment, and water quenching are excluded.

Rodriguez-Vargas et al. (Contribution 5) present a revised paper focusing on recent advances in the additive manufacturing of soft magnetic materials. They highlight the significant progress made in the field of materials science, which has enabled the development of novel materials such as high-entropy alloys (HEAs). These alloys, due to their complex chemical composition, can exhibit soft magnetic properties. The aim of the present work was to provide a critical review of the state-of-the-art SMMs manufactured through the use of different AM technologies. This review covers the influence of these technologies on microstructural changes, mechanical strength, post-processing, and magnetic parameters such as saturation magnetization (MS), coercivity (HC), remanence (Br), relative permeability (Mr), electrical resistivity (r), and thermal conductivity (k).

Zhao et al. (Contribution 6) describe the evolution of the microstructure, precipitation behavior, and mechanical performance of Nb-V-Ti micro-alloyed steel prepared under different tempering times, which were studied through the use of transmission electron microscopy (TEM), X-ray diffraction (XRD), and mechanical tests. It was found that the width of the martensite laths increased with the increasing tempering time. Several types of carbides, including M_3C, M_2C, $M_{23}C_6$, M_7C_3, and MC particles, were identified following tempering. The MC carbides were found to remain stable during tempering; however, the transformation behavior of other carbides was identified. The transformation sequence can be summarized as $M_3C \rightarrow M_2C \rightarrow M_7C_3 \rightarrow M_{23}C_6$. The strength was found to decrease and the Charpy impact toughness increased gradually with the increase in the tempering time. The ultimate strength (UTS) decreased from 1231 to 896 MPa, and the yield strength (YS) decreased from 1138 to 835 MPa. The −40 °C Charpy impact toughness was found to increase from 20 to 61 J as the tempering time increased from 10 min to 100 h. The evolution of carbides plays an important role in their mechanical performance.

Tan et al. (Contribution 7) report on a study examining deformed substructures including dislocation cells, nanotwins (NTs), and martensite, which were introduced into super austenitic stainless steels (SASSs) through the process of cryogenic rolling (Cryo-R, 77 K/22.1 $mJ \cdot m^{-2}$). With the reduction increasing, a low stacking fault energy (SFE)

and increased flow stress led to the activation of secondary slip and the occurrence of NTs and martensite nano-laths, while only dislocation tangles were observed under a heavy reduction via cold-rolling (Cold-R, 293 K/49.2 mJ·m^{-2}). The multiple precursors not only possess variable deformation stored energy but also experience competition between recrystallization and reverse transformation during subsequent annealing, thus contributing to the formation of a heterogeneous structure (HS). The HS, which consists of bimodal-grained austenite and retained martensite simultaneously, showed a higher yield strength (~1032 MPa) and a greater tensile elongation (~9.1%) than the annealed coarse-grained Cold-R sample. The superior strength–ductility and strain hardening observed originate from the synergistic effects of grain refinement, dislocation, and hetero-deformation-induced hardening.

Efzan et al. (Contribution 8) report on Al-10Sr alloy and Na_2CO_3 addition to LM6 (reference alloy) as hybrid modifiers through ladle metallurgy. Microstructure enhancement was analyzed through the use of an optical microscope (OM). The results were further confirmed through the use of a scanning electron microscope (SEM) and energy dispersive X-ray (EDX) spectroscopy. The results showed that Na_2CO_3 and Al-10Sr alloy successfully hybrid modified the sharp needle-like eutectic Si into fibrous eutectic Si. Soft primary Al dendrites were also discovered following hybrid modification. The formation of β-Fe flakes was suppressed, and α-Fe sludge was transformed into Chinese script morphology. A 2.13% density reduction was also recorded. A hardness test was additionally performed to examine the mechanical improvement of the hybrid modified LM6. A reduction in hardness of 2.3% was recorded in the hybrid modified LM6 through ladle metallurgy. Brittle cracks were not observed, while ductile pileups were the main features that appeared on the indentations of hybrid-modified LM6, indicating a brittle-to-ductile transformation after hybrid modification of LM6 by Na_2CO_3 and Al-10Sr alloy through ladle metallurgy.

Liu et al. (Contribution 9) adopted an elastoplastic phase field model to investigate the influence of external loading on the martensitic phase transformation kinetics in steel. The phase field model incorporates external loading and plastic deformation. During the simulation process, the authenticity of the phase field model is ensured by introducing the relevant physical parameters and comparing them with experimental data. During the calculations, loads of various magnitudes and loading conditions were considered. An analysis and discussion were conducted concerning the volume fraction and phase transition temperature during the phase transformation process. The simulation results extensively illustrate the preferential orientation of variants under different loading conditions. This model can be applied to the qualitative phase transition evolution of Fe-Ni alloys, and the crystallographic parameters adhere to the volume expansion effect. The authors of the study concluded that uniaxial loading promotes martensitic phase transformation, while triaxial compressive loading inhibits this process. From a dynamic perspective, the authors demonstrate that external uniaxial loading accelerates the kinetics of martensitic phase transformation, with uniaxial compression being more effective in accelerating the phase transformation process than uniaxial tension. When compared to experimental data, the simulation results provide evidence that, under the influence of external loading, the martensitic phase transformation is significantly influenced by the applied load, with the impact of external loading being more significant than that of plastic effects.

He et al. (Contribution 10) present a review paper examining constitutive models for the strain strengthening of austenitic stainless steels at cryogenic temperatures. In this paper, the mechanical properties and microstructure evolution of austenitic stainless steels under different temperatures, types, and strain rates are compared. The phase-transformation mechanism of austenitic stainless steels during strain at cryogenic temperatures and its influence on strength and microstructure evolution are summarized. The constitutive models of strain strengthening at cryogenic temperatures were set to calculate the volume fraction of strain-induced martensite and predict the mechanical properties of austenitic stainless steels.

Chu et al. (Contribution 11) analyzed the precipitation behaviors of Ni-Cr-Co-based superalloys with different Ti/Al ratios aged at 750, 800, and 850 °C for up to 10,000 h using scanning and transmission electron microscopy. The Ti/Al ratio did not significantly affect the diameter of the γ' phase. However, the volume fraction of the γ' phase increased with the increase in the Ti/Al ratios. The η phase was not observed in alloys with a small Ti/Al ratio; however, it was precipitated after aging at 850 °C for 1000 h in alloys with a Ti/Al ratio greater than 0.80. Higher aging temperatures and higher Ti/Al ratios led to faster η formation kinetics and accelerated the degradation of alloys. It is thought that the increase in hardness with an increase in the Ti/Al ratio is attributed to the effective inhibition of the γ' phase on dislocation movement due to the increase in the volume fraction of the γ' phase and an increase in the antiphase boundary (APB) energy.

Wang et al. (Contribution 12) report on porous tantalum (Ta) implants with important clinical application prospects due to their appropriate elastic modulus and excellent bone growth and bone conduction ability. Ta microstructure designs generally mimic titanium (Ti) implants commonly used in the clinic, and at present, there is a lack of research on the influence of such microstructures on the mechanical properties and penetration characteristics, both of which will significantly affect bone integration performance. The authors of this study explored the effects of different microstructure parameters, including the fillet radius of the middle plane and top planes, on the mechanics and permeability properties of porous Ta diamond cells through simulation and put forward an optimization design with a 0.5 mm midplane fillet radius and a 0.3 mm top-plane fillet radius in order to significantly decrease the stress concentration effect and improve permeability. On this basis, the porous Ta structures were prepared through the use of laser powder bed fusion (LPBF) technology and evaluated before and after microstructural optimization. The results showed that the elastic modulus and yield strength increased by 2.31% and 10.39%, respectively. Concurrently, the permeability of the optimized structure also increased by 8.25%. It should be noted that the optimized microstructure design of porous Ta has important medical application value.

Hernandez-Flores et al. (Contribution 13) report on austenitic stainless steel ER308 coating on H13 tool steel through the use of the robotic GMAW process. The heat input during the process was calculated to establish a relationship between the geometry obtained in the coating and its dilution percentage. Furthermore, the evolution of the microstructure of the coating, interface, and substrate was evaluated through the use of XRD and SEM techniques. Notably, the presence of martensite at the interface was observed. The mechanical behavior of the welded assembly was analyzed through Vickers microhardness, and a pin-on-disk wear test was employed to assess its wear resistance. It was found that the dilution percentage is around 18% at high heat input (0.813 kJ/mm) but then decreases to about 14% with reduced heat input. Microhardness test results revealed that at the interface, the maximum value is reached at around 625 HV due to the presence of quenched martensite. Moreover, increasing the heat input favors wear resistance.

Lee et al. (Contribution 14) studied the phase separation in Al–Ti–Cu–Co alloys through use of the spark plasma sintering process. A lightweight Al-Ti-containing multi-component alloy with excellent mechanical strength and an Al–Ti–Cu–Co alloy with a phase-separated microstructure was prepared. The granulometry of metal particles was reduced using planetary ball milling. The particle size of the metal powders decreased as the ball milling time increased from 5 to 7 and up to 15 h (i.e., 6.6 ± 6.4, 5.1 ± 4.3, and 3.2 ± 2.1 μm, respectively). The reduction in particle size and the dispersion of metal powders promoted enhanced diffusion during the spark plasma sintering process. This led to the micro-phase separation of the (Cu, Co)2AlTi (L21) phase, and the formation of a Cu-rich phase with embedded nanoscale Ti-rich (B2) precipitates. The Al–Ti–Cu–Co alloys prepared using powder metallurgy through spark plasma sintering exhibited different hardness values of 684, 710, and 791 HV while maintaining a relatively low density of 5.8–5.9 g/cm^3 (<6 g/cm^3). The mechanical properties were improved upon due to a decrease in particle size achieved through increased ball milling time, leading to a finer grain

size. The L21 phase, consisting of (Cu, Co)2AlTi, is the site of basic hardness performance, and the Cu-rich phase is the mechanical buffer layer between the L21 and B2 phases. The finer network structure of the Cu-rich phase also suppresses brittle fracture. These results are important and useful for innovative applications or high process temperatures where extreme requirements are necessary for the tool material and innovative tool concept.

Klančnik et al. (Contribution 15) investigated the effects of small boron additions on the solidification and microstructure of hypo-eutectic alloyed gray cast iron. The characteristic temperatures upon crystallization of the treated metal melt were recorded with regard to small boron addition through the use of thermal analysis with the ATAS system. Additionally, a standardized wedge test was performed to observe any changes in chill performance. The microstructures of the thermal analysis samples were analyzed using a light optical microscope and field emission scanning electron microscope equipped with an energy-dispersive spectroscope, which revealed the variation in graphite count number with boron addition within the examined random and undercooled flake graphite. The effect of boron was estimated through the use of classical analytical and statistical approaches. The solidification behavior under equilibrium conditions was predicted through a thermodynamic approach using Thermo-Calc. Based on all gathered data, a response model was set with boron for a given melt quality and melt treatment using the experimentally determined data. The results of the study revealed that boron as a ferrite- and carbide-promoting element under the experimental conditions shows weak nucleation potential in synergy with other heterogenic nuclei at increased solidification rates; however, no considerable changes were observed in the TA samples solidified at slower cooling rates, indicating the loss of overall inoculation effect. The potential presence of boron nitride as an inoculator for graphite precipitation for a given melt composition and melt treatment was not confirmed in this study. From the results of the above study, it would seem that boron at increased solidification rates can contribute to overall inoculation; however, at slower cooling rates, these effects are gradually lost and in the last solidification range at increased boron content could have a carbide-forming nature, as usually expected. The results of this study suggest that boron in trace amounts could affect the microstructure and properties of hypo-eutectic alloyed grey cast iron.

Wang et al. (Contribution 16) employed molecular dynamics simulation with a cooling rate of 2×10^{10} for $Cu_{100-X}FeX$ (where X represents 1%, 3%, 5%, and 10%) alloy to explore the crystalline arrangement of the alloy and the processes involving iron (Fe) precipitation. The results showed that when the Fe content was 1%, Fe atoms consistently remained uniformly distributed as the temperature of the alloy decreased. Furthermore, there was no Fe atom aggregation phenomenon. The crystal structure was identified as FCC-based Cu crystal, and Fe atoms existed in the matrix in solid solution form. When the Fe content was 3%, Fe atoms tended to aggregate with the decrease in the temperature of the alloy. Moreover, the proportion of BCC crystal structure exhibited no obvious changes, and the crystal structure remained as FCC-based Cu crystal. When the Fe content was 5% and 10%, the Fe atoms exhibited obvious aggregation with the decreasing temperature of the alloy. At the same time, the aggregation phenomenon was found to be more significant with higher Fe content. Fe atom precipitation behavior can be delineated into three distinct stages. The initial stage involves the gradual accumulation of Fe clusters, characterized by a progressively stable cluster size. This phenomenon arises due to the interplay between atomic attraction and the thermal motion of Fe-Fe atoms. In the second stage, small Fe clusters undergo amalgamation and growth. This growth is facilitated by non-diffusive local structural rearrangements of atoms within the alloy. The third and final stage represents a phase of equilibrium where both the size and quantity of Fe clusters remain essentially constant following crystallization of the alloy.

Yang et al. (Contribution 17) studied the structure and properties of Ti_nB_n (n = 2–12) clusters and simulated the microstructure of the Al-Ti-B system through molecular dynamics to determine the grain refinement mechanism of Al-Ti-B master alloy in Al alloy. Based on the density functional theory method, the structural optimization and

property calculations of Ti_nB_n (n = 2–12) clusters were carried out. The clusters at the lowest energy levels indicate that the Ti and B atoms were prone to form TiB_2 structures, and the TiB_2 structures tended to be on the surface of the clusters. The $Ti_{10}B_{10}$ cluster was determined to be the most stable structure in the range of n from 2 to 12 in relation to average binding energy and second-order difference energy. The analysis of HOMOs and LUMOs suggested that TiB_2 was the active center in the cluster and the activity of Ti was high; however, the activity of B atoms decreased as the cluster size n increased. In contrast, the prediction of reaction sites using the Fukui function, condensed Fukui function, and condensed dual descriptor showed that Ti atoms were more active than B atoms. Furthermore, the TiB_2 structures were found in the Al-Ti-B system simulated by the ab initio molecular dynamics method, and it was found that there were Al atoms growing on the Ti atoms in the TiB_2. Based on the above analysis, the results of this study suggested that TiB_2 may be a heterogeneous nucleation center of α-Al. This study helps to further understand the mechanism of Al-Ti-B-induced heterogeneous nucleation in Al alloys, which can provide theoretical guidance for related experiments.

X. Li et al. (Contribution 18) report on porous $Ni_{50}Mn_{28}Ga_{22}$ alloy produced through powder metallurgy, with NaCl serving as the pore-forming agent. The phase structure, mechanical properties, and magnetic properties of annealed bulk alloys and porous alloys with different pore sizes were analyzed. Vacuum sintering or mixed green billets in a tube furnace was employed, which facilitated the direct evaporation of NaCl, resulting in the formation of porous alloys characterized by a complete sinter neck, uniform pore distribution, and a consistent pore size. The authors of the study found that porous alloys within this size range exhibit a recoverable shape memory performance of 3.5%, as well as a notable decrease in the critical stress required for martensitic twin shear when compared to that of bulk alloys. Additionally, porous alloys demonstrated a 2% super-elastic strain when exposed to 353 K. Notably, under a 1.5 T magnetic field, the porous Ni50Mn28Ga22 alloy with a pore size ranging from 20 to 30 μm exhibited a peak saturation magnetization of 62.60 emu/g and a maximum magnetic entropy of 1.93 J/kg·K.

G. Morettini et al. (Contribution 19) present a study undertaken in response to two instances of unexpected blade breakage in the cutting blade used in a Carton Wrap machine (CW). Failure of the Al7075 alloy blade occurred at an indentation, during typical operational loading conditions. Subsequent metallographic examinations of the fractured samples confirmed that both cases were attributed to fatigue failure. The main objective of this study was to investigate potential causes of fatigue failure in the CW blade using simplified linear elastic static numerical simulations through finite element analysis (FEA). In this research, the well-established theory of critical distance (TCD) was employed and the authors provided its contextualization at an industrial level for the specific case of the cutting blade. Furthermore, the analysis focuses on a second key aspect: proposing a new blade geometry aimed at mitigating the identified issues and eliminating possible causes of failure. In this context, the actual stress concentration at the indentation is determined using the theory of critical distance with the linear method (ML). The results from the numerical simulations indicate that the new blade geometry significantly reduces the stress concentration, resulting in a risk factor reduction of approximately four when compared to the original blade design, even under non-optimal operating conditions. Overall, the proposed numerical approach, in conjunction with simple linear static FEA, provides substantial support for designers, especially in fault analysis and when comparing different industrial solutions.

R. Dong et al. (Contribution 20) report on the effect of deformation degree on the microstructure and properties of nickel-base alloys for forgings. They describe an experiment using a free-forging hammer to achieve a deformation degree ranging from 60% to 80%. The impact of the forging deformation degree on the hardness and high-temperature erosion performance was evaluated using the Rockwell hardness tester (HRC) and high-temperature erosion tester, respectively. The experimental results indicate that as the deformation degree increased, the hardness of the forged material progressively increased

while the rate of high-temperature erosion gradually decreased. In order to comprehensively study the mechanism responsible for variations in forging performance, optical microscopy (OM), scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), and transmission electron microscopy (TEM) were employed. The findings reveal that as the deformation degree increased, the presence of small-angle grain boundaries and an increase in grain boundary area contributed to enhanced hardness in the alloy forgings. Furthermore, it was discovered that grain boundaries with twin orientation promoted dynamic recrystallization during deformation, specifically through a discontinuous dynamic recrystallization mechanism. Additionally, the precipitated γ' phase in the alloy exhibited particle sizes ranging from 40 to 100 nm. This particle size range resulted in a higher critical shear stress value and a more pronounced strengthening effect on the alloy.

H. Sun et al. (Contribution 21) investigated the improved high temperature stability and hydrogen penetration through a Pd/Ti composite membrane with TaTiNbZr intermediate layer. In their paper, the hydrogen separation membrane, a dense TaTiNbZr amorphous layer, was prepared between Pd and Ta to form a Pd/TaTiNbZr/Ta membrane system to prevent the reaction between Pd and Ta at high temperature. The structural stability, as well as the chemical stability of the Pd/TaTiNbZr/Ta film system at high temperatures, was investigated through annealing at 600 °C for 24 h. The high-temperature hydrogen permeation properties of the Pd/TaTiNbZr/Ta film systems were investigated through the use of hydrogen permeation experiments at 600 °C after heat treatment for 6 h. The TaTiNbZr layer was significantly hydrogen permeable. With the increase in the thickness of the barrier layer, the hydrogen permeability of Pd/TaTiNbZr/Ta decreases; however, its hydrogen permeation flux was smaller than that of the highest value of Pd/Ta when it reached the steady state. The presence of the TaTiNbZr layer effectively blocks the interdiffusion between Pd and Ta to form TaPd3, thus improving the sustained working ability of the Pd/TaTiNbZr/Ta membrane system. The results of this study show that TaTiNbZr is a candidate material for the intermediate layer to improve the high-temperature stability of metal–composite hydrogen separation membranes.

L. Bajtosova et al. (Contribution 22) investigated the sintering dynamics of nickel nanoparticles (Ni NPs) through a comprehensive approach that included in situ transmission electron microscopy annealing and molecular dynamics simulations. In this study, the authors systematically examined the transformation behaviors of Ni NP agglomerates over a temperature spectrum from room temperature to 850 °C. The experimental observations, supported by molecular dynamics simulations, revealed the essential influence of rotational and translational motions of particles, especially at lower temperatures, on sintering outcomes. The effect of the orientation of particles on the sintering process was confirmed, with initial configurations markedly determining sintering efficiency and dynamics. The calculated activation energies observed in this investigation follow those reported in the literature, confirming surface diffusion as the predominant mechanism driving the sintering of Ni NPs.

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