Data-driven Design of Rhenium-free Ni-based Superalloy and its Additive Manufacturing by an Electron Beam

Introductory part, Abstract: A state-of-the-art trend in developing superalloys with high performance and low cost is to avoid the use of elements such as rhenium and ruthenium whereas sustaining desirable high-temperature mechanical properties. Based on the philosophy of materials genome engineering and our previous work, this collaborative research is to establish a methodology of data-driven design of one Rhenium-free Nickel-based superalloy and its additive manufacturing by electron beam.

From June to August in 2019, Prof. Deng Pan from Shanghai University visited Prof. Akihiko Chiba group to further their collaboration on development of advanced metallic materials and their applications by electron beam additive manufacturing (EB-AM). To be more specific, the two groups aims at developing a methodology of data-driven design of a superalloy processed by EB-AM. During his stay, Prof. Pan worked closely with Prof. Chiba and his group members including Drs. Huakang Bian and Qisheng Li, Mr. Lingxiao Ouyang on development of relevant techniques such as high-throughput fabrication and processing of alloy powders. As a result of this visit, two collaborative proposals have been successfully submitted to National Science Foundation of China (NSFC) and Japan Science Promotion Society (JSPS), respectively, in 2020.

Nickel-based superalloys (NBS) contain carefully balanced alloying additions of chromium, cobalt, aluminium, titanium and other elements and have been widely used in applications of turbine blades in air turbine engines for power generation, aircraft and marine propulsion.

It is well known that use of rhenium in the NBS greatly improves the creep resistance at high temperatures, hence the in-service temperature, of the alloy. However, formation of topological close-packed phases (TCP) in company of the rhenium addition in the NBS embrittles the superalloy at room temperature. In addition, sparse reserves as well as high cost of alloying elements such as rhenium and ruthenium significantly hinder their potential in material selection for future designs of turbine engine components. In consequence, a state-of-the-art trend in developing alloys with a combination of high performance and low cost for turbine blades is to avoid the use of elements such as rhenium and ruthenium whereas sustaining desirable high-temperature mechanical properties such as superior creep resistance and excellent oxidation resistance. Moreover, availability of performance evaluation and properties data of the alloys are of essential importance to ensure the reliability of turbine engines. Nevertheless, conventional 'trial & error' approach appears to slow down the progress in search of more advanced NBS as a result of the complexity in alloy composition and extremely long and costly design cycles.

The philosophy of Materials Genome Initiative (MGI) first proposed by Barack Obama in 2012 has been widely implemented in recent years to accelerate the discovery, design, development and deployment of new, advanced materials by employing high-throughput computational selection, machine learning and high-throughput synthesis/characterization techniques. For example, Liu *et al* designed an amorphous alloy system (Ir-Ni-Ta-(B)) with a glass transition temperature of 1162K and strength of 3.7GPa at 1000K by high-throughput MGI engineering, which significantly improves the properties of other bulk metallic glasses and conventional high-temperature alloys [1].

Additive manufacturing (AM) is defined as the process of joining materials to make parts from 3D model data, usually layer upon layer, as opposed to subtractive and formative manufacturing methodologies became a research highlight in the world in recent years. Electron beam melting (EBM) as one AM technology have been used in aerospace and medical fields because EBM can produce the product directly with complex shapes and excellent quality materials. The interest of industry in EBM technology is increasing year by year.

By in-depth discussions and preliminary efforts by Prof. Pan and Chiba group, a few key scientific and technological issues have been sorted out for successful implementation of this joint research:

i) the strengthening mechanism(s) by solid solutions in the complex and multicomponent superalloys without Rhenium addition, which may be hinged to a) the interaction among alloying elements in the multicomponent alloy, and b) the interaction between the alloying elements and defects such as dislocations and stacking faults.

ii) The phase transformation in solid-liquid and liquid-liquid interfaces during melting and solidification processes of Rhenium-free superalloy by electron beam 3D printing.

iii) High temperature measurements of mechanical properties of small-sized superalloys.
4. to optimize the reversed design parameters (processing windows) for one material and fast yet reliable microstructural characterization during electron beam 3D printing.

In turn, combination of first principle calculations and machine learning, machine learning prediction models of substitutional energy of alloying elements will be established and trained for prediction of substitutional energy and local geometry of NBS and the occupying tendency of alloying elements in multicomponent system: a) different elements in the same phase (γorγ′); and the same element in different phases (γandγ′); b) different elements in the same defect (dislocation or stacking fault); and the same element in different defects (dislocation and stacking fault); c) the same element in different phases and defects; d) microstructural and stoichiometric analysis of model alloys.

More than 10 compositions will be expectedly proposed for fabrication of alloy powders by casting followed by atomization for 3D printing. Millimeter-sized specimens will consequently be produced by 3D printing, the processing parameters of which will be rapidly and effectively optimized employing in-house high-throughput technique of single-channel electron beam melting (3-5 scanning for each of 5*5 specimens) (Fig. 1) and machine learning prediction.

The temperature-dependent mechanical properties (e.g. elastic modulus, yield strength, creep) of the small-sized specimens will be characterized by high temperature microsample uniaxial tensile testing and stress relaxation with a designed temperature range from ambient to 900 °C. The strain measurement of tiny specimens is implemented via a non-contact interferometric technique based on Young's two-slit interference principle. The reliability, accuracy and effectiveness of the resulting data-mining and artificial intelligence paradigm will be validated and optimized.

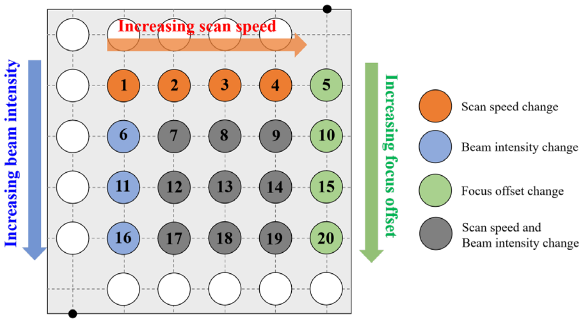

Fig.1 shows a high-throughput electron-beam additive manufacturing technique at Chiba group for batch fabrication and processing optimization of small size samples.

References

[1] Li MX, Zhao SF, Lu Z, et al. Nature (2019), 569(7754): 99.

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