

High-throughput characterization method of non-equiatomic high entropy alloys

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ABSTRACT

High entropy alloys (HEAs) are alloys with a novel design concept that, in contrast to conventional alloys, consists of multi-principal elements. Several systems investigating these unexplored chemical compositions have already been proven to be very interesting materials both as structural and functional materials. The development of new HEAs represents a great challenge, since the number of possible combinations of principal elements explodes with the complexity of the alloy. It is still trickier when investigating non-equiatomic compositions and the possibility of minor alloying additions. Computational methods such as the CALPHAD method have been successfully used to assess numerous systems, but these methods rely heavily on thermodynamic databases that are currently incomplete for the majority of HEA systems. Moreover, these methods predict phase stability but do not allow the estimation of the mechanical properties [1].

An experimental approach to screen the vast composition range of HEAs is the “diffusion multiple approach” [2]. This method consists in heat-treating at high temperature an assembly of metal blocks to activate the diffusion and consequently creating gradients of compositions. Chemical and physical properties can then be directly probed within a defined area owing to characterization methods such as EDX and EBSD. Furthermore, mechanical properties can be assessed using nanoindentation. Coupling diffusion multiples with the CALPHAD method and the modelling of nanoindentation is thus a powerful approach for the accelerated design of high-entropy alloys.

A preliminary diffusion multiple design has been thoroughly characterized to assess this approach. The diffusion multiple consisted in three blocks, Co-Ni, Fe-Mn and Cr, assembled by hot pressing after polishing the contact surfaces. The sample was then heat-treated at 1000°C for 24h. Following EBSD and EDX characterization, several zones with promising morphologies were selected and probed by nanoindentation (figure 1). From those results, the composition Cr₄₅Mn₁₆Fe₂₃Ni₈Co₈ (at%) was selected and cast for further characterization.

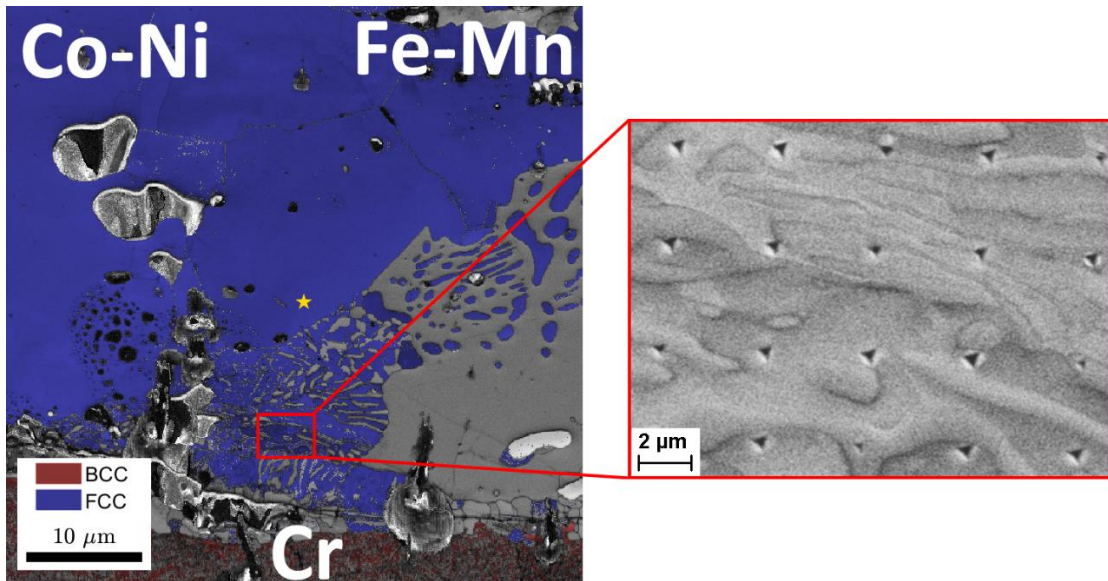


Figure 1: Band contrast and phase map close to the triple junction of the diffusion multiple. The yellow star has the equiatomic of the well-studied CrMnFeCoNi HEA. The red rectangle corresponds to a zone of interest probed with nanoindentation.

References

- [1] D. Miracle, B. Majumbar, K. Wertz, and S. Gorsse *New strategies and tests to accelerate discovery and development of multi-principal element structural alloys*, Scripta Materialia, **127**, pages 195-200, 2017
- [2] J.C. Zhao, M.R. Jackson and L.A. Peluso, *A diffusion multiple approach for the accelerated design of structural materials*, MRS bulletin, **27** (4), pages 324-329, 2002