



Short communication

Phase-evolution in high entropy alloys: Role of synthesis route



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ABSTRACT

Synthesis route can have a significant influence on the process of phase-choice and -evolution in High Entropy Alloys (HEAs). With the objective of instituting awareness, this communication on the foundation of phase diagrams, adopted using the CALPHAD approach, attempts at describing and deciphering the cause for such gradation.

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1. Introduction

Of late, the concept of the high entropy alloys (HEAs) has mustered substantial importance in the research community. In theory, HEAs differs from the primordial and rest of present-day materials, in that their genesis is believed to be governed primarily by entropy. HEAs are therefore defined to be systems having multi-principal elements in equimolar ratio or with concentrations between 5 and 35 at. % [1]. Amongst other fields relating to HEAs, the largest dedication has been towards realising their phase evolution, and microstructural designing. While some HEAs have been reported to take complex and random atomic structures -intermetallics, amorphous-, a majority of these are single or the mixture of simple solid solutions [2]. A number of models are today at our disposal to predict the phase-type that a HEA microstructure may grab, majority of which are thermodynamics based.

HEAs are commonly being synthesized via three routes [3,4]: Powder Metallurgical (Mechanical Alloying), Casting (Arc Melting, Die Casting, Induction Melting), and Deposition (Plasma Spraying, Sputtering); the choice among which, however is less scientific. Interestingly, amidst such full-blown research, what seems missing is an observation towards HEAs showcasing different

microstructures under varied processing techniques. An understanding towards differing phase-evolution phenomenon is of utmost importance since the material properties are a function of microstructure, and deviation from the expected could be disturbing.

That given, in the light of this communication, an explanation for this mysterious behaviour with CoFeNi, CoCuFeNi, and CoCrFeNi as examples, is attempted on the basis of thermodynamic approximation, so that a universal understanding is instituted. The results corroborate to have a long reach in research concerning synthesis and designing of HEAs.

2. Results and discussion

Thermodynamic phase stability of the systems as a function of chemical composition and temperature has been modelled using the CALPHAD (CALculation of PHase Diagrams) approach, which has been adopted through Thermocalc software (TCFE7 and SSOL4 database). Interestingly the BCC-B2 phase has not been incorporated in both TCFE7 and SSOL4 databases of the Fe-Co binary system. In the present work authors have calculated the phase diagram by invoking the thermodynamic description for BCC-B2 phase in Fe-Co system. Table 1 features the crystal structure, and method of synthesis, reported for these selected CoCuFeNi and CoCrFeNi HEA alloys. As is evident from Table 1, in either system, a variance in the crystal structures as a function of synthesis route can be noted.

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Table 1
Variation in the crystal structures as a function of synthesis route.

System	Synthesis route	Phase type	Reference
CoCuFeNi	Induction Melting	FCC1(Major) + FCC2(Minor)	[5]
	Mechanical alloying	FCC	[6]
CoCrFeNi	Mechanical Alloying	FCC(Major) + BCC(Minor)	[3,7]
	Die casting	FCC	[8]
CoFeNi	Mechanical Alloying	FCC	[3]
	Induction Melting	FCC	[5]
	Die casting	FCC	[8]

We postulate that the digression in the choice of crystal structure follows from the starting state of the material, used in synthesis. While in casting and deposition (spraying) process, the starting state is a liquid, in the powder metallurgical route, that state is a solid. This simple classification has a significant impact, in that the sequence of phase-evolution turns upside down. In the former, evolution in phase is a result of cooling, against the latter, where the modus operandi is heating. In better terms, one moves from top to bottom across a phase diagram in liquid-state processing routes, and vice versa in the solid-state process of powder metallurgy.

Fig. 1a and b illustrates the phase diagram of CoCuFeNi and CoCrFeNi alloys respectively. According to phase diagram, FCC is the first phase to nucleate from the liquid in either system (CoCuFeNi and CoCrFeNi), and as has been observed multiple times experimentally, it tends to remain unaltered, despite continuous cooling to room temperature (Table 1). This is intriguing as it is well-known that phase transformation can be a strong function of cooling and heating rates. Therefore, it is expected here that the FCC phase

transforms to low-temperatures phases –in accordance to phase diagram–, on slow-cooling, as imposed by Die-Casting, or Induction Melting. Interestingly however, despite such slow cooling rates, FCC remains common to both systems (Table 1), remaining unchanged when the starting state is liquid. This eccentric behaviour could be best explained by the sluggish diffusion effect [9]. In brief, phase transformation during solidification requires distribution of elements, which often is a collective movement. But the differences in the local atomic arrangement, due to varied neighbouring atoms, and the varying diffusion capability among elements, coupled together, can severely obstruct such arrangements, i.e. material freezes to the first solid-state it assumes.

This behaviour is expected to multiply in deposition routes like the plasma spraying, where the cooling rates are much greater. This phenomenon of sluggish diffusion while explaining the passive effect from heating/cooling rates, puts forward a theory that the first phase to nucleate from liquid has the highest probability to be retained at room temperature unless equilibrium conditions are inflicted. Our trails on randomly chosen HEAs (Table 2), add weight to this postulation. This suggests that the system's choice for a phase, when the starting state is liquid, could be predicted, in advance, from phase diagrams, which can be generated through easy-to-use softwares like ThermoCalc, Pandat, Factstage etc.

For the HEAs developed from the solid-state process of Mechanical alloying, the phase evolution is towards a direction pointing upwards on the phase diagram. While it is certainly true that the mechanical alloying process is a non-equilibrium process, it needs to be understood that under non-contaminating conditions, the options on phases are not infinite, and that the choice is greatly inclined towards those observed in equilibrium phase diagrams. In fact, at most occasions, binary phase diagrams, and the

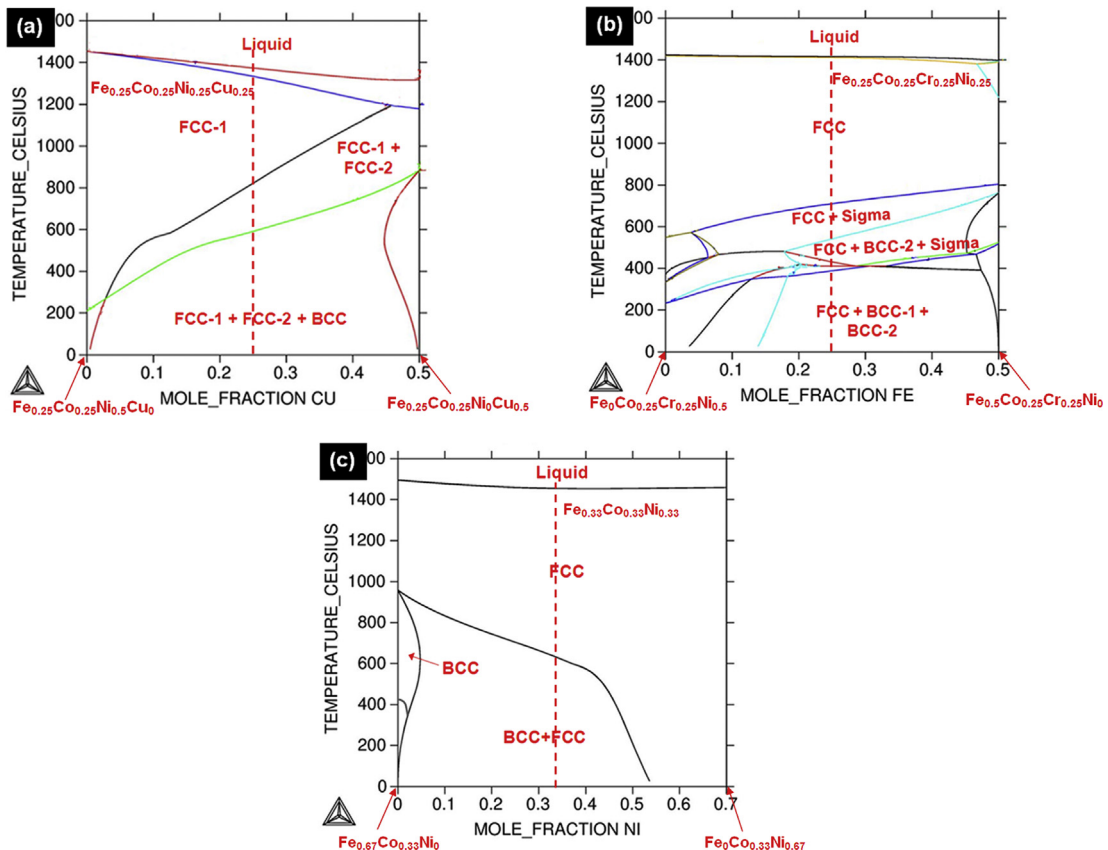


Fig. 1. Vertical Section of (a) CoCuFeNi, (b) CoCrFeNi and (c) CoFeNi phase diagrams, generated using the CALPHAD approach.

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