Comprehensive study of complex metallic and multi-component alloys using electron crystallography methods

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Engineering of non-expensive alloys with perfect combination of physical properties were always the Holy Grail of materials engineering. Two paths were chosen by our group to achieve this goal: study of ternary systems where new intermetallic phases have been discovered and development of novel multi-component alloys (often called high entropy alloys (HEAs)).

Since structure and properties are interlinked, study of atomic structure is prerequisite for understanding the properties. Structure solution of intermetallics is not a trivial task. These materials often have narrow homogeneity regions which limit the possibility of the growth of a single crystal. In most of the cases, powder X-ray diffraction cannot be used for the solution of these structures, as their lattice parameters are quite high, and they crystallize as nano-sized precipitates in metallic matrices together with additional, crystallographically related phases. Furthermore, contrary to other complex materials, the atomic distances and angles of intermetallics are not fixed and their coordination polyhedra are usually unknown which makes it harder to validate the solution of their structure. It these cases, electron crystallography (EC) methods are the only viable tool. However, their application is not trivial as dynamical effects in the data, taken from these structures, are highly pronounced which hinders the solution and refinement. The contribution of our group to the development of routine structure solution path for aluminides (as an example of intermetallics) was summarized in [1,2]. Since then, we have succeeded in solving many structures of ternary aluminides using 3D electron diffraction (3D ED) methods. In all cases, the symmetry of the unit cell was evaluated using Convergent Beam ED methods enabling not only estimation of the extinction/diffraction symbol but determination of the full space group symbol, differentiating between the centrosymmetric and non- centrosymmetric space groups. The uniqueness of our approach is in combination of data and methods. We often obtain the information from both direct and reciprocal space and cross reference between them for verification, compare obtained data to simulation of direct and/or reciprocal space and/or to other related structures.

As to the second path – we focused on AlCoCrFeNi, as it is an example of the BCC-based family of HEAs which exhibits superior strength and good corrosion resistance [3]. In addition, owing to its high Al and Fe contents, the AlCoCrFeNi alloy is lighter and cheaper than conventional superalloys. One of the major disadvantages of this alloy is the formation of the σ phase at intermediate temperatures, which embrittles the alloy and hampers its commercialization [4]. Several years ago, we revealed anti-phase boundaries (APBs) (parallel to $\{110\}$ planes) in the B2 (ordered BCC) matrix of the AlCoCrFeNi [4,5]. Periodic APBs have suppressed the phase transformation to the unwanted brittle σ phase. To harness this effect, thorough study of the APBs in B2 structure was performed. In general, APB is a planar defect which might form in ordered superlattices. This defect has been thoroughly studied in the ordered FCC structures, $L1_2$, such as Ni_3Al [6], while research on APBs appearing in B2, has been limited. To simplify the task, AlFe was chosen following Density Functional Theory calculations as the B2 binary prototype since it exhibited the lowest APBs energy among the other binary B2 phases in the Al-Co-Cr-Fe-Ni system [7]. Furthermore, the addition of Cr and Ni to AlFe reduced the APBs energy even more [7]. Applying various EC methods, we characterized structural defects forming in the non-stoichiometric Al-Fe B2 and succeeded in formulating APBs formation mechanism [8]. It was established that the formation of APBs is closely linked to the degree of order. Raising compositional complexity, Al-Fe-T (where T=Cr, Ni) ternary alloys were studied. It was proven that Cr occupies exclusively Al sublattice, while Ni – Fe sublattice. Isolating disorder at each sublattice, it was found that only disorder at the Al sublattice encourages formation of the APBs. Attempting to control the formation of the APBs, the complexity was raised to quaternary AlCoCrFeNi and quinary AlCoCrFeNi compositions. Obtained results have validated proposed in [9] APBs formation mechanisms.

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