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Crystallographic data mining - A path to structure prediction in intermetallics?

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Many metals adapt very simple structure types, mainly sphere packings such as cubic and hexagonal close-packed, as well as simple body-centered cubic structures. In contrast, around 2 % of all intermetallic crystal structures exhibit unit cells containing 100 or more atoms [1]. These compounds are also termed "complex intermetallics" and, while the simplest packings approximate metal atoms as spheres and in doing so explain a number of frequent structure types, the existence of such intricate geometries is not immediately evident. From the analysis of a large number of intermetallic structures, we can recognize geometrical patterns (e.g., recurring building blocks) in order to find out more about their general building principles. Among complex intermetallics, two very distinct phenomena can be observed when inspecting the different structures. On one hand, chemically very diverse compounds can crystallize in rather similar structures, as was shown for a group of more than 40 complex face-centered cubic compounds [2]. On the other hand, small compositional changes within select intermetallic systems can yield a number of different structures, which can also belong to the class of complex intermetallics. A showcase system is found among Al-Cu-Ta, where a small range of the ternary phase diagram contains at least four different structures, all of them complex [3]. By gaining deeper knowledge of the factors influencing structure stabilization, we aim at a better understanding of the mechanisms that are responsible for the formation of intermetallic structures. Thus, we hope to contribute to the quest for explaining why certain intermetallic structures form, while countless other theoretically possible structures do not. Consequently, the prediction of intermetallic structures, especially in still largely unknown parts of multinary phase diagrams, will come into reach.

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