

Statistics of intermetallic compounds

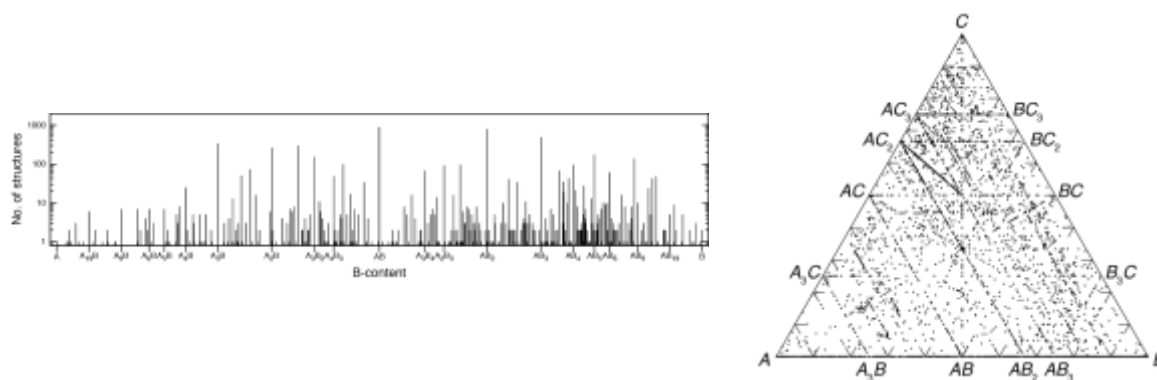
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Previously, we started investigating the dataset of the 20 829 known intermetallic structures with basic statistical methods in order to characterize “complex intermetallics” in a robust and meaningful way [1,2]. Their unit cells are large – containing 100 or more atoms. However, we discovered that – symmetry-wise – complex intermetallics do not differ from intermetallic compounds in general. Their compositions are usually not ratios of small integer numbers, as is the case with simpler structures, and certain elements occur more frequently among complex structures.

In order to be able to classify and understand complex intermetallics better, we have to learn more about all intermetallic compounds. Pettifor, among others, has attempted to find recurring patterns in the occurrence of specific structure types in intermetallics [3]. In addition to considering the elements forming different types of structures, we also analyze, *e.g.*, the stoichiometries, which form compounds at all. We try to detect regularities from the binary [4] and also ternary compositions in intermetallic systems that have been recorded so far [2]. Some interesting statistics will be presented and examples for important and complex structures will be discussed in more detail.



Compositions of the 6441 binary (*left*) and 13026 ternary (*right*) intermetallics; extracted from the 20 829 unique intermetallic compounds contained in *Pearson's Crystal Data*.

[1] J. Dshemuchadse, W. Steurer, MRS Proceedings 1517 (2012).

[2] P. Villars, K. Cenzual, *Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds*, Release 2012/13, ASM International®, Materials Park, Ohio, USA.

[3] D. Pettifor, *Bonding and Structure of Molecules and Solids*, Oxford University Press (1995).

[4] J. Dshemuchadse, W. Steurer, *Inorg. Chem.*, *submitted* (2014).