

Poster Presentations

[MS36-P01] Intermetallic structures: Constituents, Compositions, and Complexity.

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The structures of intermetallics are generally regarded as being simple and belonging to a few easily-understood structure types. However, throughout the different intermetallic and crystal systems, numerous complex structures can be found that contain hundreds or thousands of atoms in one unit cell, amounting up to the record structure in the Al–Cu–Ta-system with more than 23 000 atoms in one unit cell [1]. Among the most complex structures, mainly highly symmetric compounds of very diverse intermetallic constitutions can be found [2]. With respect to translational and point-symmetry, the occurrence of complex intermetallics resembles that of all intermetallic phases [3]. Now we are examining the distribution of different intermetallic compounds over the compositional space. For this we extract all structural data on intermetallics contained in a database for analysis [4]. The fact that preferred compositions occur at ratios of small integer numbers is broadly accepted and closely resembles the constitution of molecules. But what is the mechanism behind more intricate compositions: are the respective “metallic molecules” simply larger? Is it actually possible to identify the respective building units within the metal structure? How do coordination polyhedra and clusters in general evolve over a compositional range? Always bearing in mind the characteristics of complex intermetallics, we will try to approach these questions and uncover systematics within the realm of the structure formation of intermetallic compounds. Ultimately, nothing less than the ability to purposefully search for desired structures containing specific elements could be the aim of such a knowledge basis, i.e. “materials design” in the form of an anticipation of functional structures and – ideally

– their subsequent synthesis.

[1] Weber, T., Dshemuchadse, J., Kobas, M., Conrad, M., Harbrecht, B., Steurer, W. (2009). *Acta Cryst.* **B65**, 308-317.

[2] Dshemuchadse, J., Jung, D. Y., Steurer, W. (2011). *Acta Cryst.* **B67**, 269-292.

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

[4] Villars, P., Cenzual, K. Pearson's *Crystal Data*, Release 2012/13.

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