Poster Presentations

[MS14-P01] Structure Motif Simulation for Intermetallic Ni_2In Superstructures. Carola J. Müller, S.

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Superstructures of the NiAs-Ni2In structure family are formed by a variety of compounds that are of technical importance for batteries, semiconductors, solders and other electrical equipment.
The Ni2In aristotype structure ($P6_3/mmc$, $Z = 2$) consists of three fully occupied crystallographic positions: the hcp network unit on Wyckoff site 2*c*, the octahedral void on Wyckoff site 2*a* and the trigonal bipyramidal void on Wyckoff site 2*d*.[1] The aristotype describes a disordered arrangement. As a function of temperature and time, different atoms on same Wyckoff positions start to order in a diffusive process, and extra reflections occur as diffuse bumps before they become sharp Bragg reflections of newly formed superstructures. Unsurprisingly, the majority of Ni2In superstructures are highly pseudohexagonal. In addition to a necessary symmetry reduction, occasionally modulation wave vectors have to be introduced to describe observed diffraction patterns of an ordered superstructure as accurate as possible. So, why not building general 3+n dimensional models to simulate known and hypothetical Ni2In superstructures which can then be used to study the occurrence of the various structural motifs and their chemical consequences?

[1] Lidin, S. (1998). *Acta Cryst*. **B54**, 97-108.

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