

Editorial

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The directed synthesis of new and especially metastable solids is still a great challenge despite promising developments of synthesis techniques and characterization methods. A solid compound is formed in two principal steps: the nucleation which is followed by crystallization. Because a deeper understanding of the fundamental structure forming steps occurring during the birth of a solid compound is lacking, crystallization as a way of rational synthesis of new solids is (nearly) impossible. According to results of theoretical calculations many new solid compounds should be (kinetically) stable within a certain temperature and/or pressure regime. But as mentioned above, the primary steps at the very early stages of compound formation are not known thus preventing the synthesis of most of these theoretically predicted solids. Such new compounds may possibly display unexpected and exciting properties which cannot be explored because they cannot be synthesized. Many important technological areas strongly depend on new materials with improved or even new properties.

This special issue summarizes the results obtained within the framework of a priority program funded by the German Science Foundation (SPP1415). As may be seen the program took advantage of the rapid progress and perceptions in both the in-situ analytics and advanced theoretical approaches developing an atomistic picture of the primary steps of structure formation of solids. The understanding of the formation mechanisms turned out to be of fundamental importance for advancing synthetic strategies which give control of structure forming steps in order to direct these towards the formation of metastable crystalline solids. This way, the priority program helped to overcome the apparent shortcomings in understanding the fundamental individual reaction steps during the formation of crystalline solids. Obviously, such knowledge

proved to be a prerequisite for the more directed synthesis of metastable crystalline materials.

The following areas of interest were in the focus of the priority program:

- The directed synthesis of crystalline solids.
- The full characterization of the solids with respect to structure–property relationships, relative stability of polymorphs and so on.
- The systematic study of structure formation under in-situ conditions including precursors and/or transient crystalline intermediates.
- The simulation and modeling of structure formation.
- The screening of the energy landscape including structure and property prediction of new metastable crystalline materials in the accessible pressure–temperature regime.

A central concern of the priority program was to bring together expertise from different areas as syntheses of solids, theoretical calculations and simulation and in-situ characterization techniques. The feedback between *synthesis* \leftrightarrow *theory* \leftrightarrow *in-situ* investigations over a period of 6 years has fostered a copious understanding of the formation mechanisms of solids on an atomistic level.

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