Perfect single crystals of novel chalcogenides for photovoltaics, grown by chemical vapor transport

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Chalcogenides are becoming increasingly important materials that combine ideal properties as solar absorbers with earth-abundant and low-toxic components. In particular, adamantine-type compounds, including kesterites, are currently the most promising material for fully inorganic thin-film photovoltaic technology that is free of critical raw materials and thus offers sustainable solutions. Among the materials of increasing interest are Cu-Sn-S compounds; these are Cu_2SnS_3 (mohite) and Cu_2CuSnS_4 (kuramite) apart from the defect adamantines such as $CuGaSnS_4$. In parallel, other chalcogenides, e.g. of the ABS_3 type such as $BaZrS_3$, as well as binary chalcogenides, e.g. Sb_2S_3, play an important role in the search for new materials.

When searching for new materials, perfect single crystals are indispensable when characterizing them concerning their physical and optical properties. The most suitable method for growing perfect chalcogenide single crystals is chemical vapor transport (CVT) as introduced by Nitsche [1]. With chemical vapor transport enhanced by halogens, chalcogenide crystals can be grown below critical temperatures for peritectic and eutectic points as well as for phase transitions. Growth conditions such as source temperature, temperature gradient, and transport agent concentration are important for the growth of reasonably perfect crystals. These crystals grow near thermodynamic equilibrium. The main challenge is to control the composition of the gas phase and to optimize the temperature field during growth.

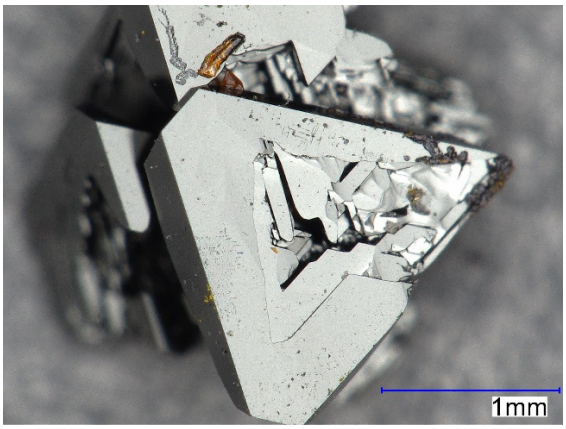

Fig.1 Single crystal of $CuAlSnS_4$

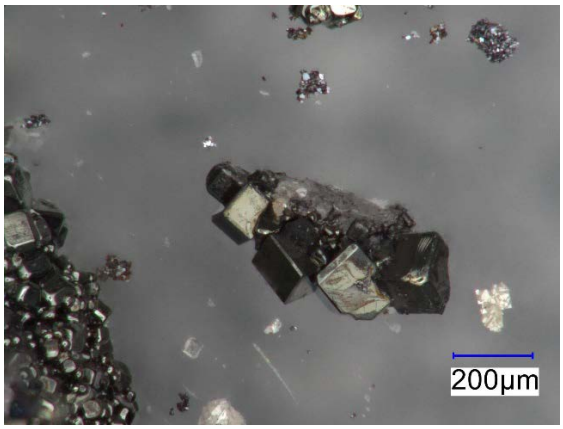

Fig.2 Single crystals of $BaZrS_3$

The crystal growth of a series of chalcogenides was studied. By varying the growth parameters of chemical vapor transport, it was possible to find out which growth conditions most influenced the quality of single crystals. In this way, the conditions for growing chalcogenide single crystals could be optimized. The grown crystals were investigated for their chemical, structural, physical and optical properties. The suitability of the analyzed materials for photovoltaics could be evaluated based on the results of the perfect single crystals.

References

[1] Nitsche, R., Fortschr. Miner., 1967, 44, 231- 287