Se-doped antimony telluride: Se sites position determination

Meledin, A.[1,2], Küpers, M.[3], Herrmann, M.[4], Stoffel, R.[3], Dronskowski, R.[3], Friese, K.[3,4] and Mayer, J.[1,2]

[1] Central Facility for Electron Microscopy (GFE), RWTH Aachen, 52074, Germany, [2] Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C), Forschungszentrum Jülich GmbH, Jülich, 52428, Germany, [3] Institut für Anorganische Chemie, RWTH Aachen, Aachen, 52074, Germany, [4] Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, 52428, Germany

Recently a lot of attention has been payed to investigations of antimony telluride: a promising candidate for non-volatile phase-change memories and thermoelectric devices applications [1]. Sb_2Te_3 is built of repeated Te2-Sb-Te1-Sb-Te2 layers (Te1 and Te2: symmetrically independent Wyckoff positions) resulting in tetradymite structure (space group *R-3m*) [2]. Adding dopants into the structure could open the doors to fine tuning the physical properties of Sb_2Te_3 - based solid solutions [3]. Se-doped antimony telluride ($Sb_2Te_{3-x}Se_x$) is isostructural to pristine Sb_2Te_3 and Se was suggested to preferably occupy the Te1 sites. However, up to now the detailed structure analysis was not reported.

A combination of HAADF-STEM with EDX mapping was applied to precisely locate Se atomic positions inside $Sb_2Te_{3-x}Se_x$ structure. The results come in good agreement and are nicely supported by structure determination based on XRD single crystals measurement performed for $Sb_2Te_{3-x}Se_x$ with x varying from 0 to 1.55 (fig. 1).

TEM investigations evidenced preferential incorporation of Se atoms mostly into Te2 positions (fig. 2). Se atoms were also observed in Te1 positions. Together with this some Se was found to take A1 sites explaining the missing electron density in single crystal measurements.

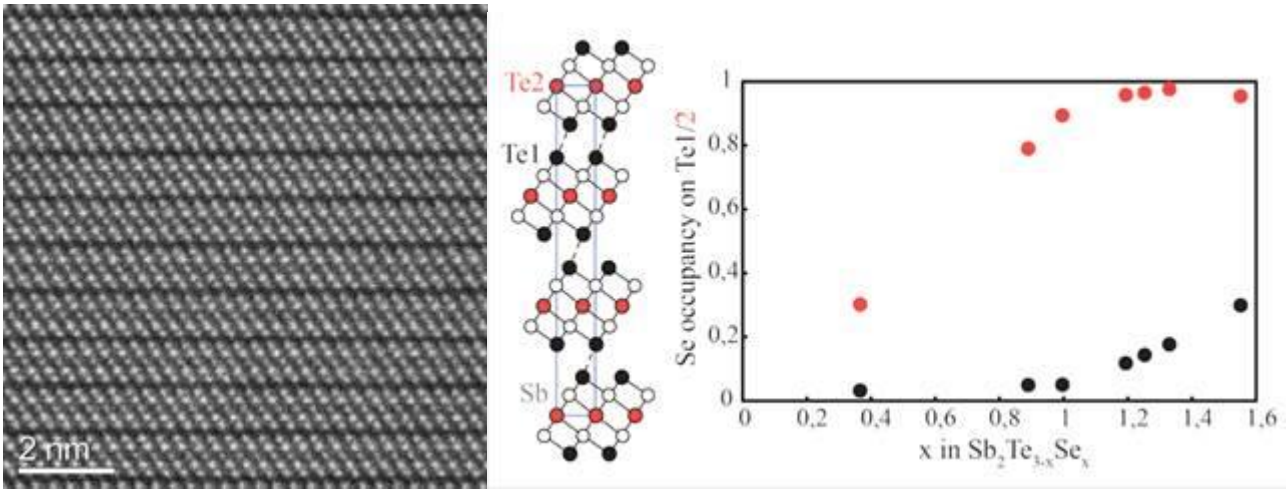

Figure 1. HR HAADF STEM image of $Sb_2Se_{1.8}Te_{1.2}$ material, illustrating its layered structure, Sb_2Te_3 structure model together graph showing the Se Te1/2 position occupation vs the Se concentration in $Sb_2Te_{3-x}Se_x$.

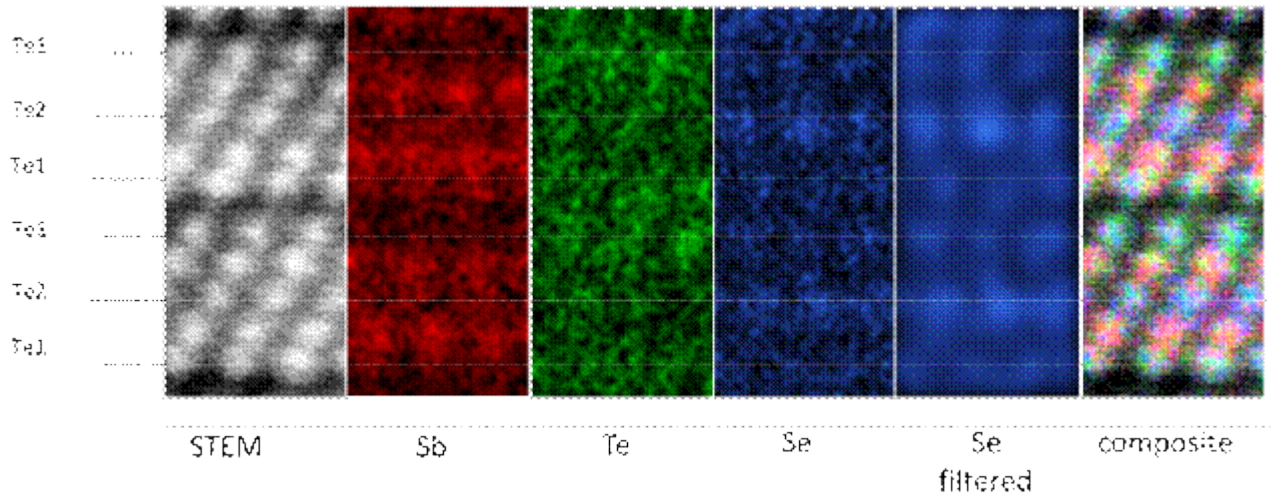

Figure 2. Atomic resolution STEM image together with elemental maps for Sb, Te and Se of $Sb_2Se_{1.2}Te_{1.8}$ compostion, showing Se atoms occupying preferentially Te2 positions.

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