Contribution ID: **158** Type: **Talk (20 min + 5 min discussion)**

The half- to full-Heusler transition in Ni_{1+x}MnSb

Thursday, 8 December 2022 13:40 (25 minutes)

Structural voids are a defining feature of the half-Heusler structure. Using temperature-dependent neutron diffraction, the disordering of these vacancies is followed across the $C1_b$-$L2_1$ transition in samples of $Ni_{1+x}MnSb$ for various Ni excesses x, demonstrating the second-order nature of this transition. Structure solution on high-resolution room-temperature neutron diffraction as well as X-ray diffraction data yields a vacancy content in excess of $1 - x$, the concentration of constitutional vacancies in the ideal model of site occupations. This is mirrored by the increased lattice constant during temperature-dependent diffraction on cooling, implying an annihilation of the initial vacancy excess at elevated temperatures. The reason for this very slow time-scale of vacancy concentration equilibration as compared to typical systems will be discussed, and consequences for the materials properties will be pointed out.

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