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NEUTRON DIFFRACTION STUDY OF A NON-STOICHIOMETRIC Ni-Mn-Ga MSM ALLOY

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Abstract. The structure and chemical order of a Heusler alloy of non-stoichiometric composition Ni-Mn-Ga were studied using constant-wavelength (1.538 Å) neutron diffraction at 363K and the diffraction pattern was refined using the Fullprof software. At this temperature the structure is austenite (cubic) with $Fm\bar{3}m$ space group and lattice constant of $a = 5.83913(4)$ [Å]. The chemical order is of critical importance in these alloys, as Mn becomes antiferromagnetic when the atoms are closer than the radius of the 3d shell. In the studied alloy, the refinement of the site occupancy showed that the 4b (Ga site) contained as much as 22% Mn; that significantly alters the distances between the Mn atoms in the crystal and, as a result, also the exchange energy between some of the Mn atoms. Based on the refinement, the composition was determined to be $Ni_{1.91}Mn_{1.29}Ga_{0.8}$

NOTE: The complete article can be found at <https://www.scientific.net/MSF.738-739.103>.