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Magnetic properties and stability of the atomic laminate Mn$_{2}$GaC. MARTIN DAHLQVIST, ÁRNI INGASON, Linköping University, Sweden, GUNNAR PÁLSSON, Uppsala University, Sweden, BJÖRN ALLING, IGOR ABRIKOSOV, JOHANNA ROSEN, Linköping University, Sweden — Using first-principles calculations, we predicted the thermodynamically stable magnetic Mn$_{2}$GaC and subsequently synthesized it as a heteroepitaxial thin film. It belongs to a class of atomically laminated compounds with a unique combination of metallic and ceramic properties. They have a common formula $M_{n+1}AX_n$M$_{n+1}$AX$_{n}$ (n = 1-3), where M is an early transition metal, A is an A-group element, and A is carbon or nitrogen. Using density functional theory (DFT) and Heisenberg Monte Carlo (HMC) for a magnetic ground state search, several collinear and noncollinear low energy magnetic spin configurations have been identified, some with different symmetries compared to the non-magnetic crystal structure. Around 240 K X-ray diffraction and magnetic measurements display a sharp contraction of the lattice in the c-direction coinciding with a sharp magnetic transition. Neutron diffraction measurements displays diffraction peaks consistent with long-ranged antiferromagnetic order with a repetition distance of two structural unit cells (25 {\AA}). This is consistent with theoretically predicted structural changes between different, close to degenerate, magnetic ground states, and it is the first unambiguous evidence of long ranged AFM order in MAX phase materials.

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