Complex ground state, spin waves and field induced transitions of the noncollinear antiferromagnet Mn_5Si_3

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Noncollinear spin configurations in magnetic materials gives rise to important macroscopic phenomena that can be exploited for developing future information and communication technologies. In this context the metallic compound Mn_5Si_3 is a promising material for applications due to its interesting transport and thermodynamic properties, such as the anomalous Hall conductivity [1] and the inverse magnetocaloric effect [2]. In the paramagnetic state, Mn_5Si_3 crystallizes in hexagonal space group $P6_3/mcm$ with two distinct crystallographic positions for the Mn atoms (sites Mn1 and Mn2) and it undergoes two phase transitions towards a collinear and non collinear antiferromagnetic (AFM) phase at T_{N2}=100K (AFM2) and T_{N1}=66K (AFM1), respectively [3]. The crystal structure of the AFM2 phase can be described by a centrosymmetric orthorhombic cell with space group *Ccmm*, where Mn2 divides into two sets of nonequivalent positions. In this cell, magnetic reflections follow the condition $h + k$ odd, the magnetic propagation vector is $\boldsymbol{\kappa} = (0, 1, 0)$, and only two-thirds of the Mn2 atoms acquire magnetic moments aligned parallel and antiparallel to the *b* axis of the orthorhombic unit cell. While neutron diffraction studies [3,4] and density functional theory calculations [5] are in agreement regarding the collinear spin arrangement in the AFM2 phase, in past years several contradicting spin structures have been proposed for the noncollinear AFM1 phase [3,6]. The noncollinear spin configuration of this system (AFM1 phase), is believed to be the origin of its important properties. In this work [7], we determine the magnetic exchange couplings of the AFM1 phase of Mn_5Si_3 using inelastic neutron scattering measurements and density functional theory calculations. We obtain the ground-state spin configuration and compute its magnon dispersion relations which are in good agreement with the ones obtained experimentally. Furthermore, we investigate the evolution of the spin structure under the application of an external magnetic field to demonstrate theoretically the multiple field-induced phase transitions which the system undergoes. Finally, we model the instability of some Mn magnetic moments in a frustrated environment to unveil their behavior under an external magnetic field.

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