Average magnetization and Fe hyperfine fields in Co_2FeSi-based Heusler alloys

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Half-metallic ferromagnetic alloys are indispensable for spintronic applications. There is a controversy between experiment and theory about the half-metallic nature of the Co_2FeSi Heusler alloy. Usually a generalized Slater-Pauling type (i.e. valency-controlled) behaviour of the average magnetization (theoretically 6 μ_B/f.u.) is considered as a conclusive proof. In the present study SQUID magnetic and ^{57}Fe Mössbauer measurements were performed to clarify the situation. Bulk $Co_2FeAl_{1-x}Si_x$, $Co_{1.9}Fe_{1.1}Al_{1-x}Si_x$, $Co_2Fe_{0.9}TM_{0.1}Si$ (TM=Ti,V,Cr,Mn,Co,Ni,Cu), $Co_{2-y}Fe_{1+y}Al$ and $Co_2Fe_{1\pm y}Si_{1\mp y}$ samples were prepared by induction melting. The $Co_2FeAl_{1-x}Si_x$ shows $L2_1$ crystal structure only for $x \geq 0.4$, between x=0 and 0.3 it has A2 structure (Fe–Al,Si disorder). The average magnetization of these alloys does not follow the expected Slater-Pauling trend (on the Si side saturation is observed around 5.75 μ_B/f.u.) and similar deviation is observed for the replacement of Fe by TM atom. The effect of the antisite disorder (Fe-Si) on the magnetization and Fe hyperfine parameters was determined and significant decrease in the Co magnetic moment for excess Si neighbourhood is extrapolated. The formerly reported large $\approx 6\mu_B$/f.u. magnetization for Co_2FeSi was observed only in samples having Fe excess and Si deficiency.