

First-Principles Disordered Local-Moment Study on Temperature Dependence of Spin Polarization in $\text{Co}_2\text{Fe}(\text{Ga}_{0.5}\text{Ge}_{0.5})$ Heusler Alloy

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Co-based Heusler alloys such as $\text{Co}_2\text{Fe}(\text{Ga}_{0.5}\text{Ge}_{0.5})$ (CFGG) [1,2] and Co_2MnSi (CMS) [3] have been proven as prospective ferromagnetic material in magnetoresistance (MR) devices due to its large spin polarization. However, the MR ratio is also significantly reduced at elevated temperature. One of the possible causes for this phenomenon is the degradation of intrinsic spin polarization of Co-based Heusler alloys electrodes at finite temperature. Therefore, to clarify the reduction of MR ratio, theoretical understanding of electronic structures at finite temperature is strongly required. In this work, the finite temperature effect on the spin polarization of Co-based Heusler alloys was studied on the basis of the disordered-local moment (DLM) [4] method, which combines the classical statistical physics and mean-field approximation to treat spin-fluctuation in magnetic systems. Then, electronic structures at finite temperature were obtained using density functional theory calculations with Korringa-Kohn-Rostoker method [5].

We show in Figs. 1(a) and (b) the temperature dependence of spin polarization of CFGG and CMS with ordered L_{21} and disordered B2 structures. It is found that the calculated temperature dependence of sp spin polarization of CFGG is smaller than CMS, which is consistent with the previous experimental work [1–3] that elucidates the contribution of bulk spin asymmetry (β) in CPP-GMR devices as shown in Figs. 1(a) and (b). The smaller temperature dependence of spin polarization in CFGG is due to the larger Curie temperature which may also affects sp density of states through the s - d and p - d intra-atomic orbital coupling. In addition, modulation of the Fermi level position in the half-metallic gap of CFGG and CMS within the rigid band model by electron and hole doping can improve the temperature dependence of the spin polarization, which is similar with our previous results on CMS [6]. The effect of electron and hole doping on temperature dependence in off-stoichiometric Co-rich and Fe-rich alloys is also discussed.

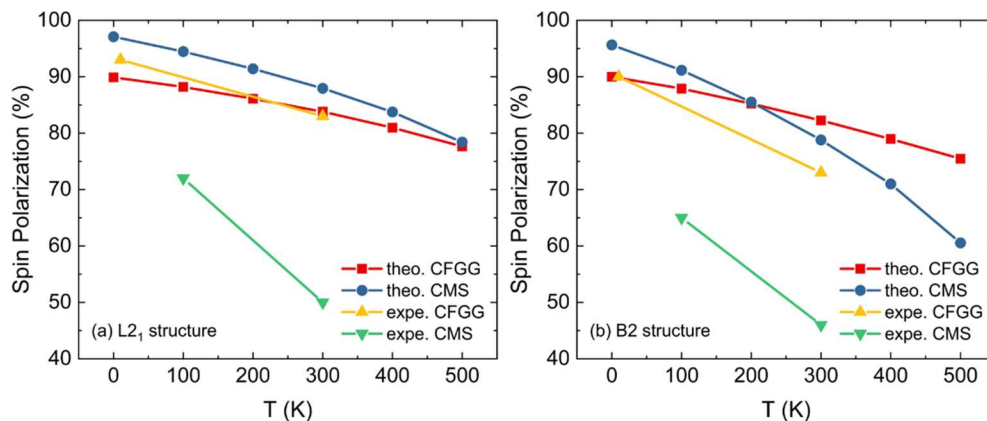


Fig. 1. Temperature-dependent spin polarization of sp states for (a) L_{21} -CFGG and CMS, and (b) B2-CFGG and CMS, denoted by “theo.” For comparison, the β values deduced from previous experiments are also shown, denoted by “expe.” L_{21} CFGG [1], B2 CFGG [2], and L_{21} and B2 CMS [3]

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