Search for New Ferromagnetic Thin Films Using Machine Learning

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In spintronics, magnetic tunnel and giant magnetoresistive junctions have been used for read heads for data storage, magnetic memories and sensors [1]. Current technology uses CoFeB as ferromagnetic layers with a face-centred cubic crystalline structure induced by a seed layer to sandwich a MgO tunnel barrier. These junctions are crystallised by post-annealing resulting in satisfying high temperature endurance (typically 1 min. at 270°C for memories and 3,000 h at 175°C for sensors) and corrosion resistance. However for further miniaturisation, a new ferromagnetic material needs to be developed with higher spin polarisation. Here, Heusler alloys hold great potential showing only one spin channel at the Fermi level, achieving 100% spin polarisation (half-metallicity) at room temperature [2], and form a pseudo-two-dimensional ultrathin film due to their layer-by-layer crystallisation with a (110) facet [3].

Machine learning was used to search for new magnetic materials in an untrathin film form with the thickness <10 nm. As an example, a NiCrMnSi [4] and CoIrMnAl [5,6] alloy films have been predicted to exhibit half-metallic ferromagnetism. These films were accordingly deposited using ultrahigh vacuum magnetron sputtering on MgO(001) and Si substrates. Their structural and magnetic properties were investigated by X-ray diffraction and transmission electron microscopy, and vibrating sample magnetometry, respectively. The optimised films were implemented in a magnetic tunnel junction for transport measurements, showing > 100% tunnelling magnetoresistance ratios at room temperature. Further optimisation on growth and annealing conditions can improve the ratio further to exceed that of commonly-used CoFeB/MgO/CoFe junctions. Our study demonstrates the usefulness of machine learning assisted by *ab initio* calculations in the search of future advanced functional materials.

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References

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