Structural and spectroscopic characterisation of heterostructures for semiconductor spintronics applications

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Spintronics is a newly emerging field that aims to utilise the spin of electrons in order to create fast and power-efficient novel logic and data storage devices [1]. Half-metal ferromagnetic (HMF) materials are crucial for spintronics since they are predicted to be to be 100 % spin-polarised at the Fermi level. One of the challenges in the field is how to preserve the predicted spin polarisation of the HMF materials when they are incorporated in nanometre scale devices, in particular at half-metal/ semiconductor interfaces. Atomically sharp interfaces with high spin polarization are indeed required for efficient spin injection. In this work, we use aberration-corrected high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) imaging, atomically resolved electron energy loss spectroscopy (EELS) and energy-dispersive X-ray spectroscopy (EDXS) measurements to study the role of structure and chemistry on the magnetic and electronic properties of the interfaces between a HMF full Heusler compound, namely $Co_2FeAl_{0.5}Si_{0.5}$, and different semiconductor substrates (Si (111) and Ge (111) respectively) onto which it was deposited [2,3].

HAADF STEM imaging shows that the structure of the CFAS films adopts a single-crystalline B2 ordering which is desirable for high spin polarisation. The CFAS films form structurally abrupt interfaces with both Si (111) and Ge (111). However spatially resolved EELS measurements reveal that although the interface is structurally abrupt, chemical intermixing occurs at the CFAS/Si (111) interface. The analysis shows the presence of $CoSi_2$ nano-islands at the interface, which are commensurate with the CFAS structure. Interestingly, first-principles calculations show that the idealised atomically sharp CFAS/Si (111) interface has an unfavourable spin-electronic configuration the spin-polarization, which can be reverted by the presence of the observed secondary interfacial phase.

In the case of CFAS grown on Ge(111) atomically sharp interfaces are also achievable with almost no strain due to the excellent lattice match between CFAS and Ge. HAADF STEM imaging and atomically resolved chemical EDX and EELS mapping show that the Ge(111) interface is realized *via* Ge-Co bonds, despite small and selective out-diffusion of Ge within a ~1 nm region of the interface. This atomic plane selective diffusion process does not change the structural integrity and spin-electronic structure of the CFAS since the out-diffused Ge selectively substitutes only Fe and Si/Al atoms, which in turn does not affect the film's half-metallicity. Despite the diffusion of Ge into the film, density functional theory calculations show that the observed chemistry and atomic structure of this interface preserve both the high spin-polarization of the CFAS film as well as its magnetic moment in the interface vicinity, making this system an excellent platform for spin-based device applications.

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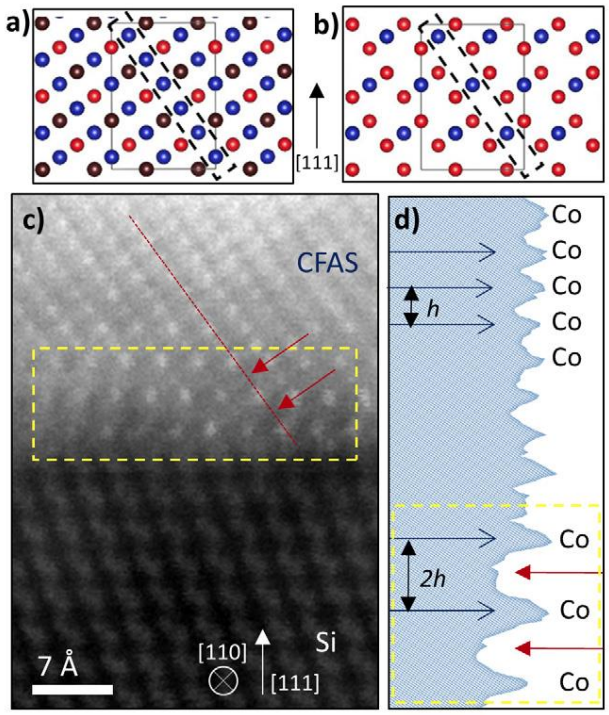

Fig. 1. Structural models for bulk (a) CFS and (b) $CoSi_2$ (viewed along the [1 1 0] direction) showing the distinctive atomic plane stacking sequence along the [1 1 1] crystallographic direction (Red balls represent Si atoms, blue Co, brown,Fe) . Dashed rectangles correspond to the red dotted line in (c). (c) HAADF STEM image of the CFAS/Si (111) interface showing the presence of the $CoSi_2$ nano-island, outlined by the yellow dashed rectangle. (d) Intensity profile along the red line in (c)[2]

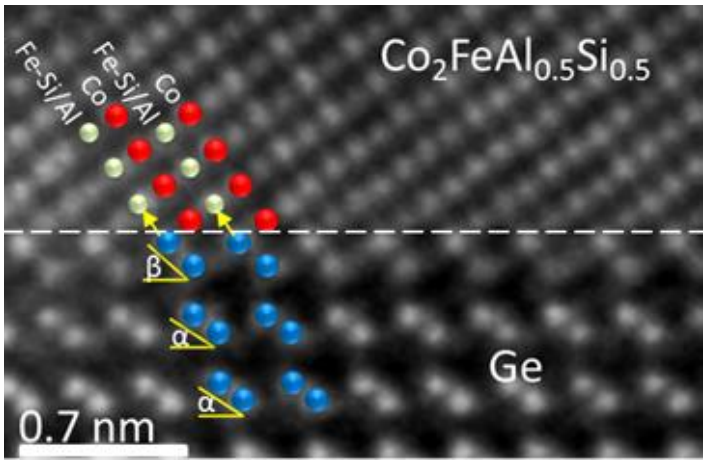

Fig. 2**:** Atomic resolution HAADF STEM image of the CFAS/Ge(111) interface showing that the CFAS film terminates on a Co(111) plane. (colour coding: Ge - blue; Co - red; Fe-Si/Al - grey). The tilt angle of the Ge dumbbells changes from α = 37° in the bulk-like region increases to β= 51° for the interfacial Ge bilayer, a result also predicted also by density functional theory [3].