doi:10.1017/S1431927616008461
Microsc. Microanal. 22 (Suppl 3), 2016

Atomic and electronic structure study of a $Co_2FeAl_{0.5}Si_{0.5}$ half-metal thin film on Si(111)

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Halfmetal/semiconductor interfaces are the key element for integration of semiconductors and magnetic materials for hybrid spintronics devices aiming at the realization of a revolutionary and energy-efficient information technology [1]. One of the biggest challenges is to directly deposit/grow halfmetal on Si, the most widely used semi-conductor substrate for these applications, due to extensive interdiffusion of the electrode elements and Si across the growth interface [2].

In this work, we study the role of chemical structure on the magnetic and electronic properties of the $Co_2FeAl_{0.5}Si_{0.5}$ (hereafter denoted CFAS) on Si(111) interface. We show that the CFAS film deposited on Si(111) has a single crystal B2 structure and forms a structurally abrupt interface with the Si substrate. Sub-nanometre resolution EELS shows that at the interface there is a mutual inter-diffusion between Si, Fe and Co over a 3 nm region. The analysis shows that this narrow interface region is Si rich and dominated by the presence of secondary $CoSi_x$ phases. Furthermore, over the same region, due to the out-diffused Si, a very faint presence of Al is detected [3].

This atomic resolution aberration-corrected electron microscopy analysis shows that the inter-diffusion is of substitutional nature, with Si mainly substituting Fe within the CFAS structure. This conclusion allows the creation of realistic models of the interface structure, used to perform further first principles calculations in order to provide insight into how the altered chemical composition modifies the local electronic and magnetic properties. The calculations show that the increased Si incorporation in the film, leads to a decrease in the magnetic moment and a significant reduction of spin-polarization at the Fermi level [3].

These effects can have a significant detrimental role on the spin injection from CFAS into Si, besides obvious consequences on the structural integrity of this junction. Therefore, these phenomena of intermixing, even though they are observed to be limited to very narrow interface region, have to be addressed and mitigated in the future in order to fully exploit the 100% spin polarization of the CFAS electrode.

References:

[1] R. A. de Groot, *et al*, Phys. Rev. Lett. **50** (1983) p.2024.
[2] M. Kawano, *et al*, Jpn. J. Appl. Phys. **52** (2013) p.04CM06.
[3] B. Kuerbanjiang, *et al*, submitted (2016)
[4] This work was funded by the Engineering and Physical Sciences Research Council (EPSRC) through grants EP/K03278X/1 and EP/K032852/1. The SuperSTEM Laboratory is the U.K. National Facility for Aberration-Corrected STEM, supported by the EPSRC.

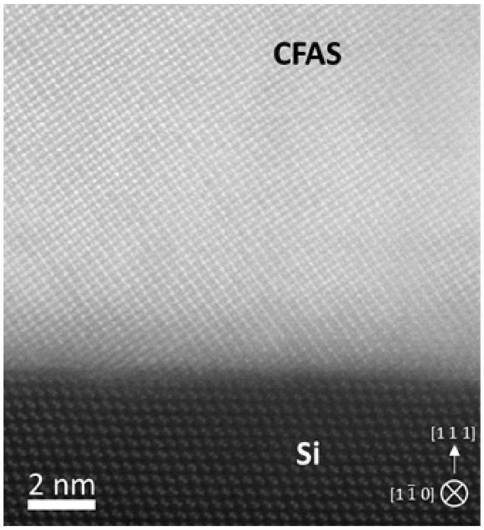

Figure 1. Atomic resolution HAADF STEM image at the interface showing the $Co_2FeAl_{0.5}Si_{0.5}$ film uniformity and structural abruptness of the interface. The imaging is performed along the Si $[1\bar{1}0]$ zone axis.

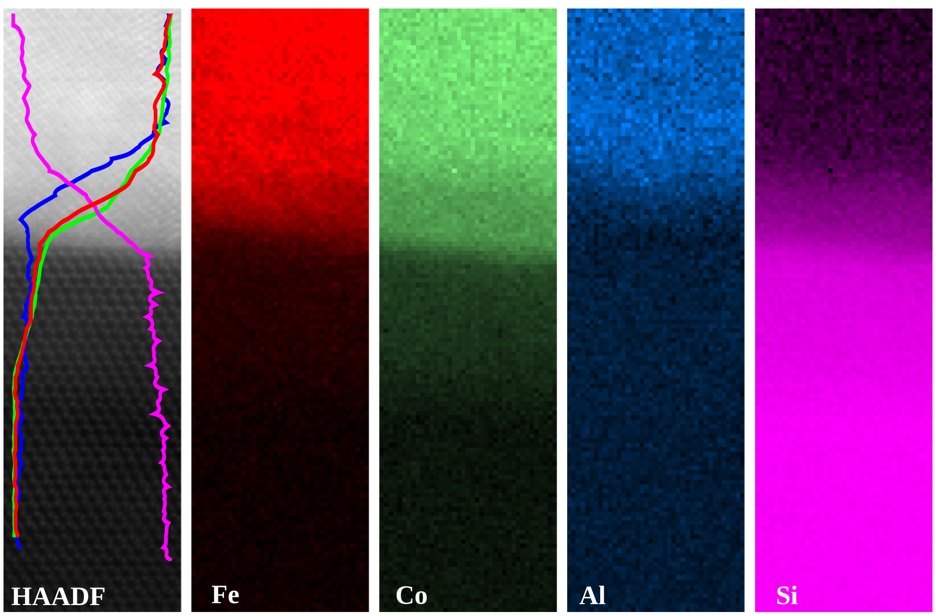

Figure 2. HAADF STEM signal and EELS elemental maps of the $Co_2FeAl_{0.5}Si_{0.5}$ /Si(111) interface showing Si inter-diffusion into the film. The integrated EELS signal of the EELS maps is plotted as line profiles against the HAADF signal.

https://doi.org/10.1017/S1431927616008461 Published online by Cambridge University Press