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# Assisting polarized neutron experimentalists: Extracting magnetic depth profiles from ab-initio calculations

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The polarised neutron reflectometry (PNR) technique measures the magnetic depth profile with nanometre-scale resolution in thin film structures. Although the raw experimental data can a rich source of qualitative information, to extract the full quantitative details, the experimentalist must solve the inverse-problem by postulating models to fit the data to yield the full set information. In PNR, this can lead to numerous free variables in the model, and unconstrained models are seldom reliable. For solid-state systems, the number of free variables can be greatly reduced by using a variety of complementary techniques including transmission electron microscopy and Rutherford back-scattering to measure the thin film chemical profile, and therefore constrain the nuclear scattering length density of the PNR model. Owing to the unique sensitivity of PNR, however, there are very few complementary experimental probes that can cross-checking the validity of the magnetic aspect of the model. For this reason, our group has developed new approaches using spin polarised DFT calculations to simulate the spin electronic density and perform averaging to mimic the PNR spatial resolution, to compare with experimental data. These ab-initio techniques only require a crystallographic starting model, and full ionic relaxation is performed in large slab models using the GADI supercomputer to reconstruct ultra-thin films (with thicknesses 1-10 nm). For thicker films, our group has explored semi-empirical models based on micromagnetic or Monte Carlo simulations where a model Hamiltonian is simulated.

This poster provide a few demonstrations of these theoretical techniques supporting PNR for studying ion-beam induced effects in exchange-biased effects in Co/Pd hydrogen sensors [1], NiFe/Fe2O3 bilayers [2] and FePt3 alloys [3].

## Speakers Gender

Male

## Level of Expertise

Experienced Research

## Do you wish to take part in the poster slam

Yes

**Primary author(s) :** Dr DAVID, Cortie (University of Wollongong)

**Presenter(s) :** Dr DAVID, Cortie (University of Wollongong)

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