## Atomistic simulations of antiferromagnets and ultrafast exchange bias switching

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Antiferromagnets were once described by Louis Néel as "extremely interesting from the theoretical viewpoint, but do not seem to have any applications". Today antiferromagnets are essential for reading the vast amounts of information stored on magnetic disk drives as a key material in magnetic read heads, yet beyond their ability to stabilize a ferromagnet through the exchange bias effect, their magnetic properties are poorly understood and still frightfully difficult to measure. Atomistic simulations have provided new and exciting insights into the properties of industrially relevant antiferromagnets such as IrMn and we are now beginning to develop a fuller understanding of their static and dynamic properties.

 $Ir_xMn_{1-x}$  alloys are especially interesting [1], as they support two, three and four sublattice antiferromagnetic spin structures, as well as a ferromagnetic Ir<sub>3</sub>Mn phase. These different phases naturally arise due to different compositions and ordering of the Mn sites, leading to a wide diversity of magnetic properties such as different Néel temperatures and effective magnetic anisotropies. Large-scale atomistic simulations have provided new insights into the microscopic origins of the exchange bias effect in CoFe/IrMn<sub>3</sub> bilayers, arising from a natural imbalance of interfacial magnetic spins leading to a small but highly stable interfacial magnetic moment responsible for the effect. Simulations are now able to account for a wide range of observed effects including coercivity, thermal and athermal training, pinned and unpinned moments and the temperature and grain size dependence of exchange bias. More recently we have found that it is possible to manipulate the exchange bias effect using ultrafast laser pulses, achieving single-shot switching of the bias direction [2]. Supported by atomistic simulations on the UK National Supercomputer ARCHER2 [3], we found that laser pulses lead to an ultrafast demagnetization of the antiferromagnet and, combined with a CoGd layer switching via a thermally induced mechanism, the interfacial exchange field leads to a resetting of the exchange bias field on an ultrafast timescale. This unexpected result is in stark contrast to spin valves where the exchange bias setting process can take several hours. In this talk I will outline the methodology for simulating the diverse properties of  $Ir_xMn_{1-x}$  alloys and present results revealing some of their exciting static and dynamic properties. I will conclude with a brief perspective on atomistic modelling of antiferromagnets and future challenges.



Figure 1: Atomistic simulations of the dynamics of IrMn/CoGd bilayers showing the granular nature of the IrMn. Ultrafast demagnetization of the Gd, Co, and IrMn sublattices, showing distinct demagnetization times for each material and the individual response of the of the IrMn sublattice magnetization of each grain showing a coherent switching process after the pulse, before achieving a stable state at longer timescales From [2].

## References

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