Ultralow-energy Mn implantation in MoS_2: non-equilibrium magnetic doping

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Abstract

Magnetic doping of transition-metal dichalcogenides offers a route toward spin-dependent phenomena in atomically thin semiconductors, but conventional growth-based approaches tend to favor incorporation of transition-metal dopants on the metal sublattice. Here, we explore ultralow-energy ion implantation as a complementary, non-equilibrium route to magnetic doping in MoS_2. Building on our recent work demonstrating controlled Mn incorporation in graphene by ultralow-energy ion implantation [1,2], we implanted Mn ions into MoS_2 at an energy of 20 eV, aiming to access dopant configurations that are difficult to obtain during crystal growth.

The implanted samples were characterized using a combination of surface-sensitive spectroscopy, momentum-resolved electronic-structure measurements, local microscopy, and magnetic spectroscopy. X-ray photoelectron spectroscopy confirms Mn incorporation at the MoS_2 surface. Synchrotron-based angle-resolved photoemission spectroscopy shows that the overall MoS_2 band structure is preserved after implantation, while the bands become broadened due to disorder. Scanning tunnelling microscopy, supported by density-functional-theory simulations, indicates that under these ultralow-energy conditions Mn incorporation is favored on the chalcogen sublattice, rather than on the Mo site typically expected for growth-mediated substitutional doping. Finally, synchrotron X-ray magnetic circular dichroism demonstrates that the incorporated Mn carries a magnetic moment, with predominantly paramagnetic behaviour and strong indications of low-temperature antiferromagnetic interactions.

These results establish ultralow-energy ion implantation as a versatile post-growth route to magnetic functionalization of MoS_2, enabling access to dopant-site configurations outside the equilibrium growth phase space. Although the present proof-of-principle study reveals antiferromagnetic rather than ferromagnetic interactions (possibly more desirable for spin-dependent transport phenomena), it opens a broad parameter space for engineering magnetic 2D semiconductors through dopant concentration, implantation energy, alternative magnetic species, and electrostatic or chemical co-doping to tune the Fermi level and the resulting exchange mechanisms.

References

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[2] R. Villarreal et al., "Achieving High Substitutional Incorporation in Mn-Doped Graphene," ACS Nano (2024). DOI: 10.1021/acsnano.4c03475.