Defect-induced magnetic phase transition in 2D semiconductor CrSBr

Fangchao Long[1,3], Mahdi Ghorbani-Asl[1], Zdenek Sofer[2], Florian Dirnberger[3], Arkady V. Krasheninnikov[1], Slawomir Prucnal[1], Manfred Helm[1,3], Shengqiang Zhou[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany*

[2] *University of Chemistry and Technology Prague, 166 28 Prague, Czech Republic*

[3] *TU Dresden, 01062 Dresden, Germany*

f.long@hzdr.de

CrSBr is rapidly gaining attention as a prominent candidate within the family of van der Waals magnetic semiconductors [1-3]. Below the Néel temperature of 132 K, the material is supposed to exhibit prototypical A-type antiferromagnetic order, as predicted by mean-field theory years ago. Recently, however, several groups reported the observation of unusual magnetic signatures indicating a second magnetic phase transition at temperatures around 40 K. In this contribution, we are going to discuss: (1) whether these signatures reflect an intrinsic property of the material or are caused by extrinsic influences; (2) if not the former, whether one can tailor the magnetic properties after growth.

We start with CrSBr single crystals synthesized by chemical vapor transport. Surprisingly, by extensive magnetization measurement utilizing SQUID magnetometry, we cannot detect the second, 40 K magnetic phase transition [4]. Our magnetometry measurements confirm the theoretically predicted magnetic phase diagram and thus demonstrate that the 40 K phase observed by other groups is not an intrinsic element of the magnetic phase diagram of CrSBr. The pure antiferromagnetic CrSBr crystals and flakes were then subjected to non-magnetic ion irradiation, which produces structural defects in the crystals in a controllable way. We observe a transition from antiferromagnetic to ferromagnetic behavior in CrSBr (see Fig. 1 below) [5]. Already at moderate fluences, ion irradiation induces a remanent magnetization with hysteresis adapting to the easy-axis anisotropy of the pristine magnetic order up to a critical temperature of 110 K. Structure analysis of the irradiated crystals in conjunction with density functional theory calculations suggest that the displacement of constituent atoms due to collisions with ions and the formation of interstitials favor ferromagnetic order between the layers. Increasing irradiation fluences gradually lowers the Curie temperature, reflecting the impact of crystalline degradation. This suggests that by finely tuning the irradiation parameters and employing precise lithography techniques, it is possible to selectively modulate induced ferromagnetism in CrSBr in terms of magnetization strength, critical temperature, and spatial distribution. However, in our opinion, the origin and nature of the second phase with a transition temperature around 40 K reported in pristine CrSBr samples by various studies still remains elusive.

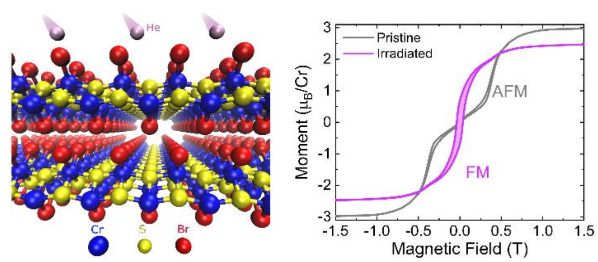

Fig.1 Ion irradiation introduces defect in CrSBr which undergoes a phase transition from antiferromagnetic to ferromagnetic.

References

[1] N. P. Wilson, K. Lee, J. Cenker et al., Nat. Mater. 20, 1657 (2021).
[2] F. Dirnberger, J.M. Quan, R. Bushati et al., Nature 620, 533 (2023).
[3] K. Lin, X. Sun, F. Dirnberger et al., ACS Nano 18, 2898–2905 (2024).
[4] F. Long, K. Mosina, et al., Appl. Phys. Lett. 123, 222401 (2023).
[5] F. Long, M.Ghorbani-Asl, K. Mosina, et al., Nano Lett. 23, 8468–8473 (2023).