Investigation of Magnetic Properties of Cr-Intercalated VTe_2

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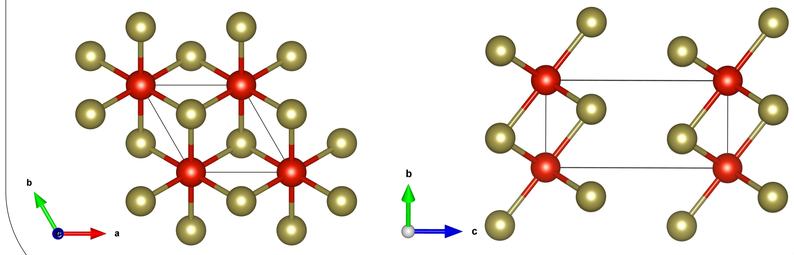
Abstract

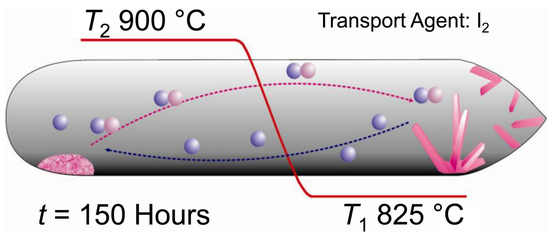
Transition metal dichalcogenides (TMDs) are layered materials with appealing magnetic and electronic. Nevertheless, in some cases, such as VTe_2, air and moisture sensitivity limits their use in real-world applications.[1-3] Intercalation of metals between the TMD layers is a viable approach to stabilizing these materials and controlling their magnetic properties.[4] In this contribution, we describe intercalation of Cr into the VTe_2 structure to yield a new crystalline phase, $Cr_{0.1}VTe_2$. We report characterization of structural and magnetic properties of this compound and theoretical calculations aimed to help with interpretation of the experimental results.

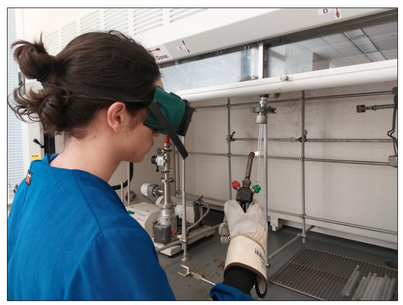


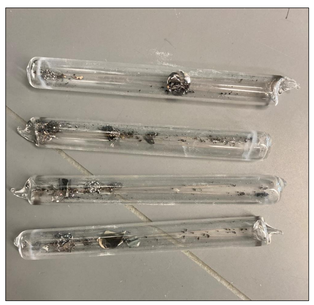
Synthesis

Synthesis of $Cr_{1/4}VTe_2$: elemental powders (Cr, V, and Te) are combined in molar ratios of 0.25:1:4.

Chemical Vapor Transport

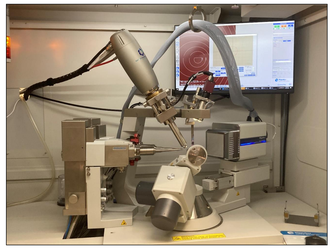






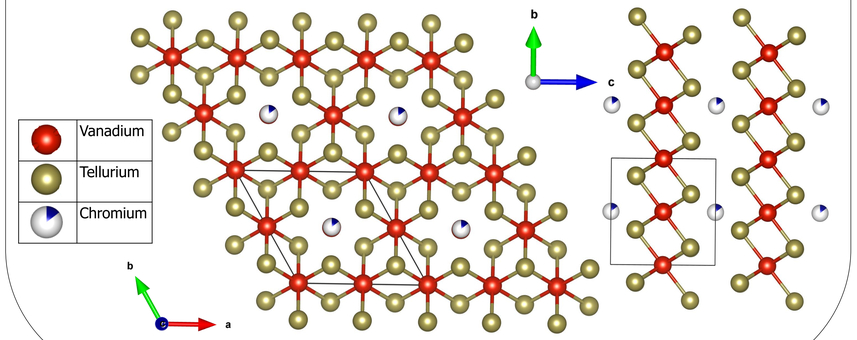
Crystal Structure

The crystal structure was determined via single crystal x-ray diffraction (XRD) on a Rigaku Synergy-S diffractometer using a Mo-K_a radiation source



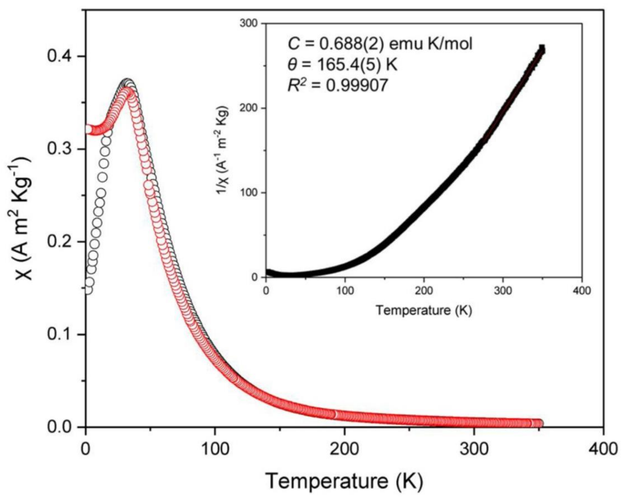
Experimental unit cell parameters

Compound	a (Å)	c (Å)	V (Å^3)
VTe_2	3.6380	6.5820	74.442
$Cr_{0.1}VTe_2$	3.7848	6.2646	77.671



Magnetic Properties

Variable temperature magnetic susceptibility measurements, performed with a superconducting quantum interference device (SQUID), reveal antiferromagnetic ordering at 32 K.



Quantum-Mechanical Calculations

Density-functional theory (DFT), FPLO (v.21-61)
8x8x8 *k*-grid, GGA-PBE functional, fully-relativistic pseudopotentials

Calculated properties of $Cr_{0.25}VTe_2$ and VTe_2

	a (Å)	*c* (Å)	*V* (Å^3)	*m*(Cr) μ_B	*m*(V) μ_B	*m*(total) μ_B	ΔE_{FM-PM} (eV/atom)
VTe_2	3.6380	6.5820	74.442	-	3.37	0.22	-0.00769
$Cr_{0.25}VTe_2$	3.6716	6.4011	74.730	3.19	1.86	2.20	-0.00196

Experimental and calculated lattice parameters show good agreement. The experimental unit cell of $Cr_{0.1}VTe_2$ is 3.0% longer in *a* and 2.4% shorter in *c* compared to the theoretically optimized structure of $Cr_{0.25}VTe_2$.

The negative ΔE_{FM-PM} (difference between energy of the spin-polarized (FM/AFM) and non-polarized (PM) configuration) indicates that magnetic ordering is favored in $Cr_{0.25}VTe_2$. The positive magnetic moments on both Cr and V sites suggest that FM ordering should be favored in $Cr_{0.25}VTe_2$, but for the experimental structure of $Cr_{0.1}VTe_2$ we observe AFM ordering.

Most likely, the material might exhibit a more complex magnetic structure with noncollinear spins due to geometric frustration.

Consistent with the behavior of other intercalated transition-metal dichalcogenides, these results suggest that $Cr_{1/4}VTe_2$ is a promising candidate for exploration of complex magnetic structures for applications in future electronic devices.

Acknowledgments & References

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1. Wasey, A. & Das, G. P. *J. Appl. Phys.* **2022**, *131*, 190701.
2. Chen, W.; Zhang, J.; Nie, Y.; Xia, Q. & Guo, G. *J. Magn. Magn. Mater.* **2020**, *508*, 166878.
3. Rajapakse, M.; Karki, B.; Abu, Abu, U.; Pishgar, S.; Musa, M.; Riyadh, S.M.; Yu, M.; Sumanasekera, G. & Jasinski, J. *NPJ 2D Mater. Appl.* **2021**, 5, 30.
4. Ahamd, & Zhou, J. *AIP Adv.* **2020**, *10*, 045323.

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