

Electronic Supplementary Information

Screw-Dislocation-Driven t -Ba₂V₂O₇ Helical Meso/Nanosquares: Microwave Irradiation Assisted-SDBS Fabrication and Their Unique Magnetic Properties

Yan Sun^{a,b}, Jianli Wang^{c*}, Mingzhe Chen^c, Chunsheng Li^{a,b*}, Zhenpeng Hu^{d*}, Shulei Chou^{c*}

^a College of Chemical Engineering, North China University of Science and Technology, Tangshan City, Hebei Province, 063009 (P. R. China)

^b Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education), Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), College of Chemistry, Nankai University, Tianjin 300071, China

Address correspondence to Chunsheng Li, lichsheng@163.com

^c Institute for Superconducting and Electronic Materials, University of Wollongong, Wollongong, NSW 2522, Australia, E-mail: shulei@uow.edu.au

^d School of physics, Nankai University, Tianjin 300071, China. E-mail: zphu@nankai.edu.cn

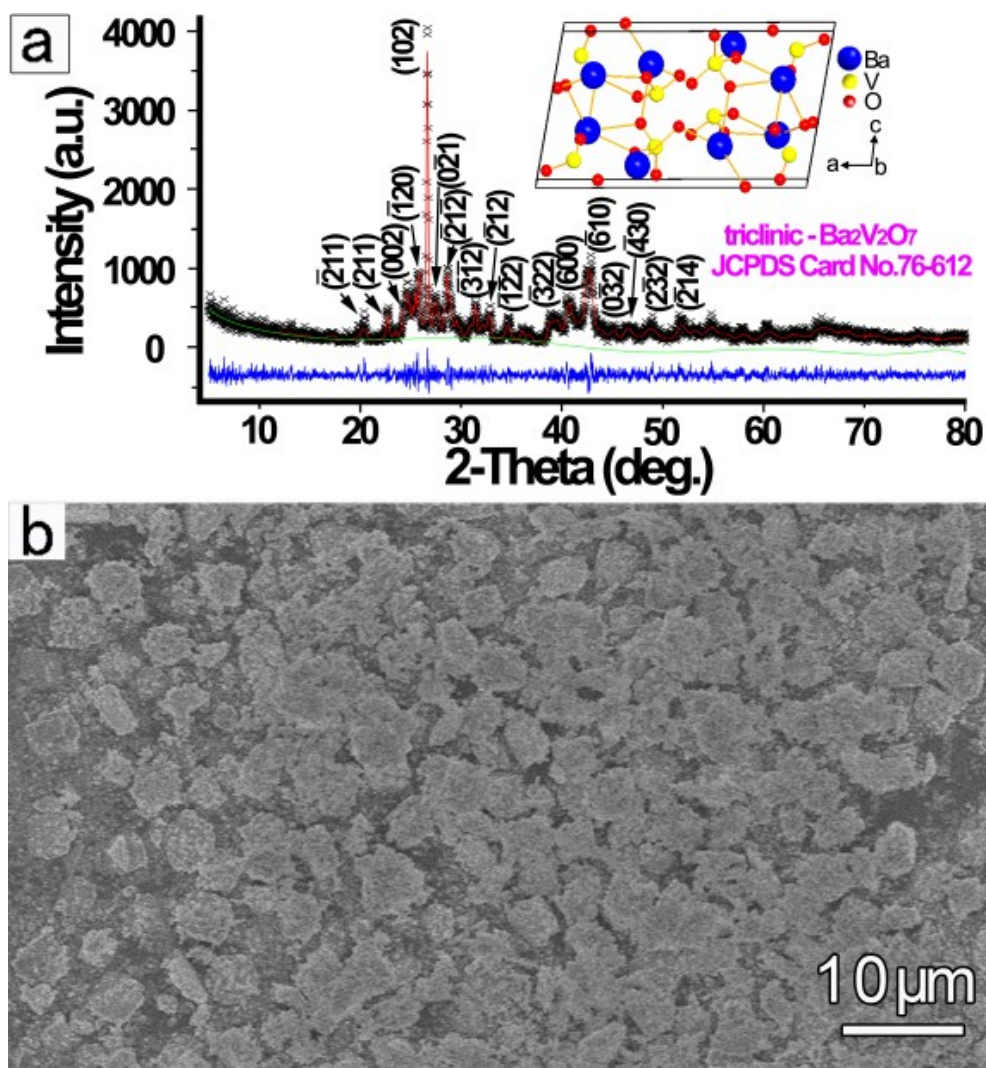


Figure S1. (a) Observed (black crosses) and calculated (red line) X-ray powder diffraction patterns of *t*-Ba₂V₂O₇ spiral-like microsquares (sample S1) revealed from simultaneous GSAS refinement analysis. The differences between the experimental and refined patterns are represented by the blue solid line at the bottom. The inset shows the crystal structure of *t*-Ba₂V₂O₇ viewed along [010]. (b) Typical SEM images of helical *t*-Ba₂V₂O₇ materials.

Table S1 Cell parameters of *t*-Ba₂V₂O₇ from refinement results of GSAS program compared with standard data.

Data	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α°	β°	γ°	R_{wp}^*	R_p^*
Refined data	13.684	7.260	7.494	89.19	100.62	88.04	0.2057	0.1571
PDF No. 76-612	13.571	7.320	7.306	90.09	99.48	87.32	-----	

Note: * R_{wp} : Reliability factor; R_p : Profile R-factor. (R_{wp} and R_p are defined in reference [1].)

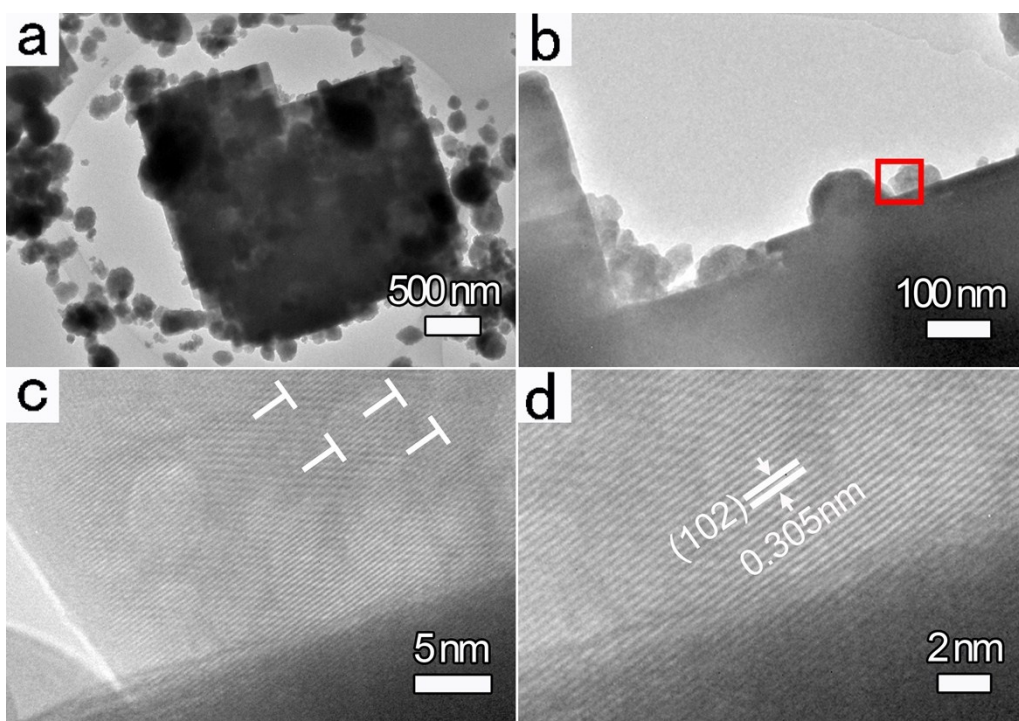


Figure S2. TEM and HRTEM images of t -Ba₂V₂O₇ helix mesostructures (sample S4), which is synthesized by microwave irradiation process via reacting for 30min. From the Figure, screw nanospheres are absorbed onto the outer surface of layered nanosquares, and control the preferential growth along 2D direction of interlaced dislocation growth.

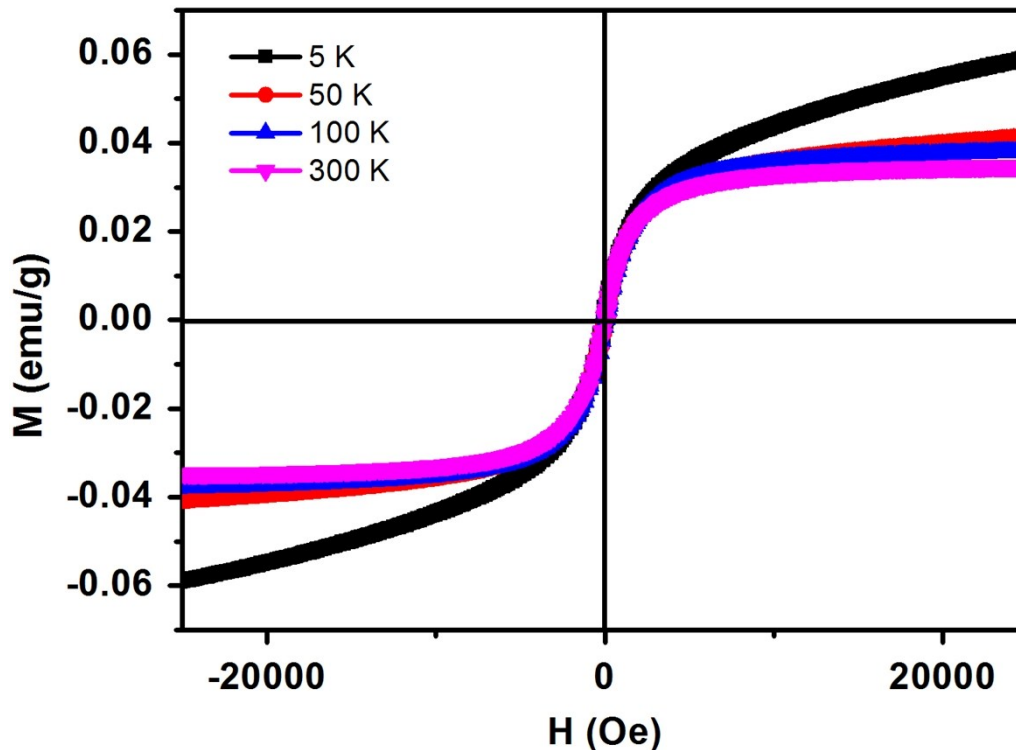


Figure S3. Magnetization curves of screw dislocated nanospheres t -Ba₂V₂O₇ (Sample S3, prepared via microwave irradiation for 2 min) as a function of the testing temperatures.

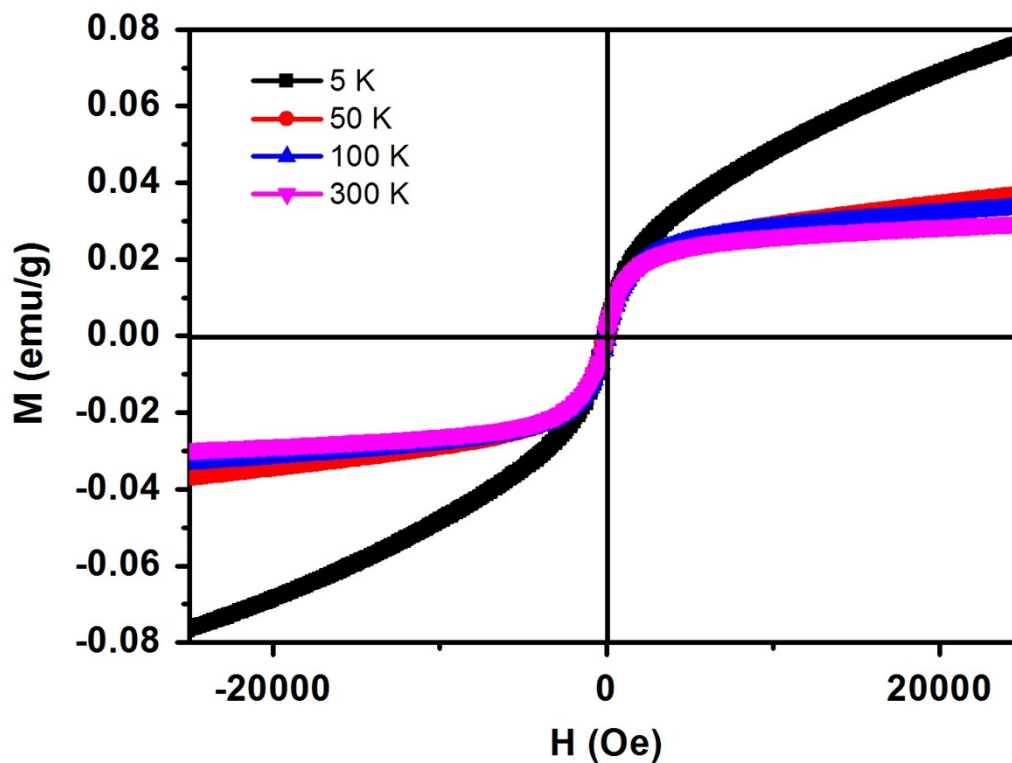


Figure S4. M–H curve of *t*-Ba₂V₂O₇ nanospheres (Sample S4, obtained by the microwave irradiation for 30 min), illustrating the magnetic properties.

Table S2 The Results of peak fitting for XPS peaks of Ba₂V₂O₇ micro/nanosquares

Sample	Valence	V ⁵⁺		V ⁴⁺		V ⁵⁺ _{2P1/2} / V ⁴⁺ _{2P1/2}
						ratio
		V _{2P3/2}	V _{2P1/2}	V _{2P3/2}	V _{2P1/2}	
XPS Sample 2	Binding energy (Standard value)	517.6		516.3		
	Binding energy	512.43	519.68	509.09	518.57	
	FWHM (eV)	0.6110	3.1951	4.9914	5.0000	
	Molar fraction (%)	0.40	72.84	14.14	12.63	5.76722

Reference:

[1] Toby, B. H. EXPGUI, a graphical user interface for GSAS. *J. Appl. Cryst.* **2001**, *34*, 210–213.