Supplementary Material

Electronic and elastic properties of metastable Zr_3N_4: a joint experimental and theoretical study

Yuhe Liu[1,2,#], Kunlun Wang[1,2,#], Nina Ge[3], Hui Sun[1,2], Bo Dai[3], Yong Wang[1,2,*]

[1] School of Space Science and Physics, Shandong University, Weihai 264209, China.

[2] Weihai Research Institute of Industrial Technology, Shandong University, Weihai 264209, China.

[3] State Key Laboratory for Environmental-friendly Energy Materials, Southwest University of Science and Technology, Mianyang 621010, China.

# These authors contribution equally.

*Corresponding author: Yong Wang: wang.yong06@sdu.edu.cn

Table S1 shows the comparison between theoretical d-space values (nm) of o-Zr_3N_4 and the values of our thin film measured by electron diffraction. The well consistency between theoretical and experimental values indicates the thin film is o-Zr_3N_4.

Table S1. The comparison between theoretical d-space values (nm) of o-Zr_3N_4 and the values of our thin film measured by electron diffraction.

(hkl)	Theoretical d values	Measured d values (ED)
310	0.310	0.309
201	0.272	0.271
410	0.237	0.238
421	0.184	0.187
511	0.165	0.166

Table S2 shows the experimental hardness values and Young's modulus of ZrN and o-Zr_3N_4 thin films. The hardness values of ZrN and o-Zr_3N_4 thin films are approximately 19.26 GPa and 7.90 GPa, which are close to the calculated hardness values of ZrN (18.06 GPa) and o-Zr_3N_4 (6.98 GPa). At the same time, the experimental Young's moduli (314.53 GPa for ZrN and 171.54 GPa for o-Zr_3N_4) also agree with the calculated results (385.86 GPa for ZrN and 212.56 GPa for o-Zr_3N_4). The consistency between experimental values and calculated results indicates the accuracy of the calculations.

TABLE S2. The experimental hardness values and Young's modulus of ZrN and o-Zr_3N_4 thin films.

	ZrN		o-Zr_3N_4	
	H (GPa)	E (GPa)	H (GPa)	E (GPa)
1	19.67	314.76	6.88	156.06
2	21.29	316.19	7.60	182.18
3	20.22	342.17	8.15	168.15
4	16.40	255.41	8.21	174.53
5	18.73	344.12	8.67	176.78
Average	19.26	314.53	7.90	171.54

FIG. S1 shows the orbital-projection electronic band dispersion of ZrN calculated by VASP and DS-PAW. Both orbital-projection electronic band dispersion show consistent features that some bands cross the Fermi level and these bands are dominated by the Zr-4*d* character, indicating that the electrons in ZrN are mainly derived from Zr-4d electrons.
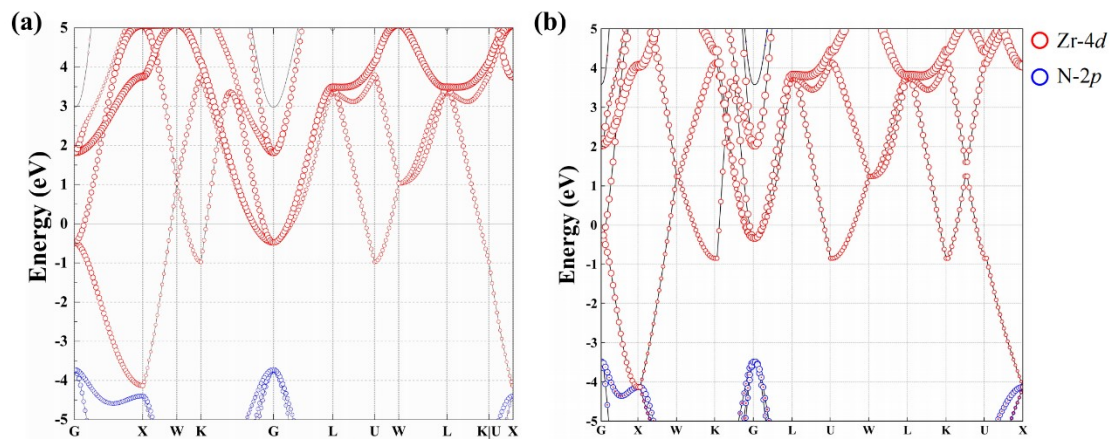

FIG. S1. The orbital-projection electronic band dispersion of ZrN calculated by (a) VASP and (b) DS-PAW.