

The Role of Interface Defects on Phase Selection in ZnO/MgO Core/Shell Nanowires

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INTRODUCTION

- ZnO nanowires have significant optical and electronic properties, which are enhanced in core-shell wires
- As shown in Figure 1 MgO can be grown epitaxially on ZnO nanowires.
- When experiments were repeated MgO grew in a polycrystalline manner as seen in Figure 2
- The growing conditions had been altered.
- Initial thoughts on the reason were oxygen vacancies on the surface

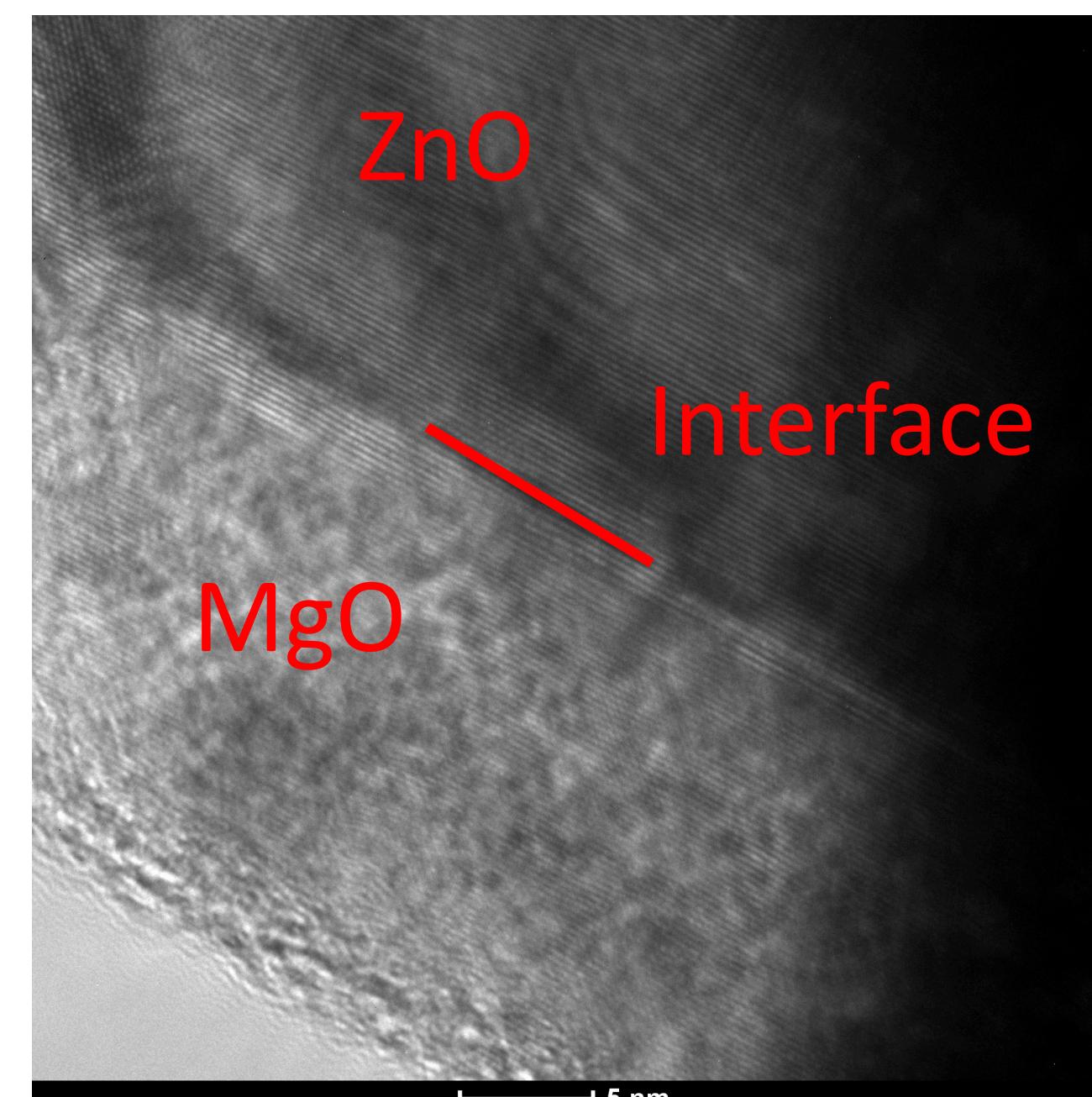


Figure 1: Epitaxial Growth of MgO onto ZnO Nanowire

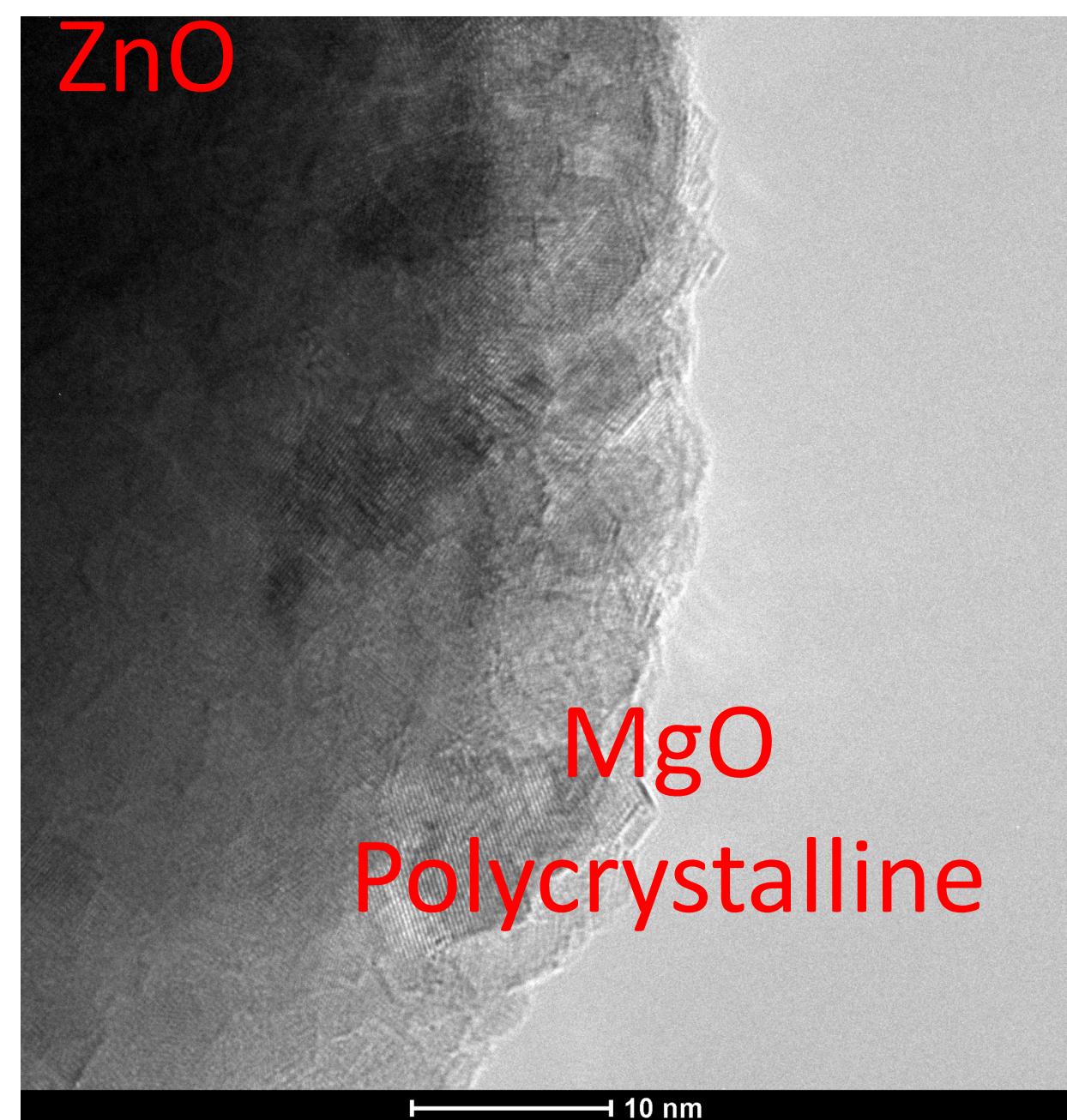


Figure 2: Polycrystalline Growth of MgO onto ZnO Nanowire

METHODS

- First principle calculations were performed on different configurations of oxygen vacancies on the interface of ZnO and MgO
- Density Functional Theory (DFT) was used to perform calculations
- DFT solves the Schroedinger many-body equation

$$\hat{H}\Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N) = E\Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N) \quad (1)$$

- DFT uses electron density rather than individual coordinates[1]

$$\Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N) \rightarrow \rho(\vec{r}) \quad (2)$$

- DFT makes these calculations possible

STRUCTURE

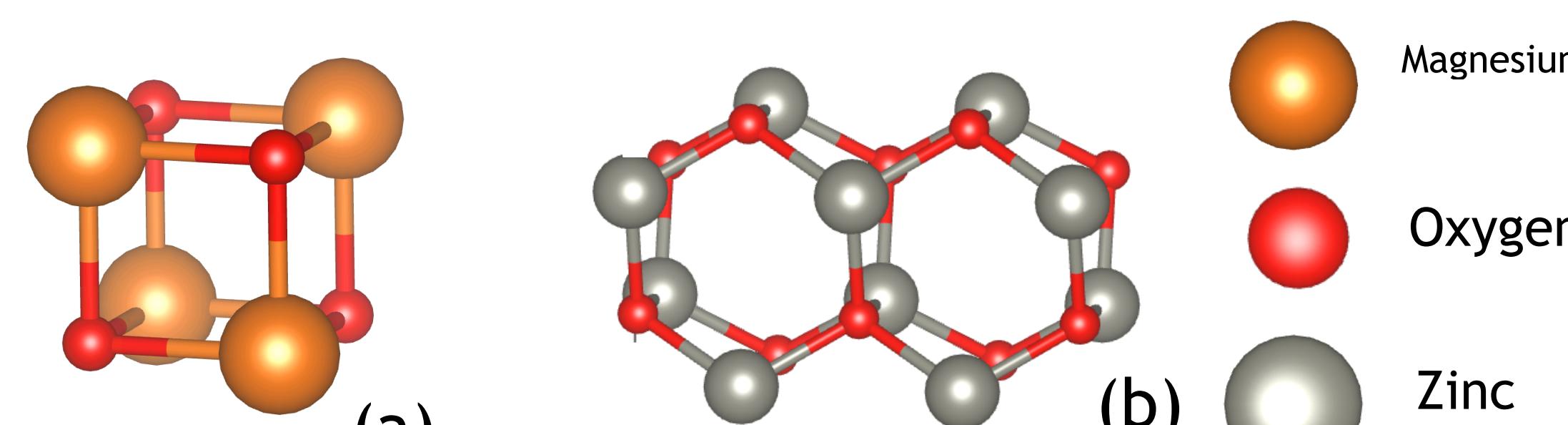


Figure 3: (a) MgO Rocksalt crystal configuration (b) ZnO Wurtzite crystal configuration

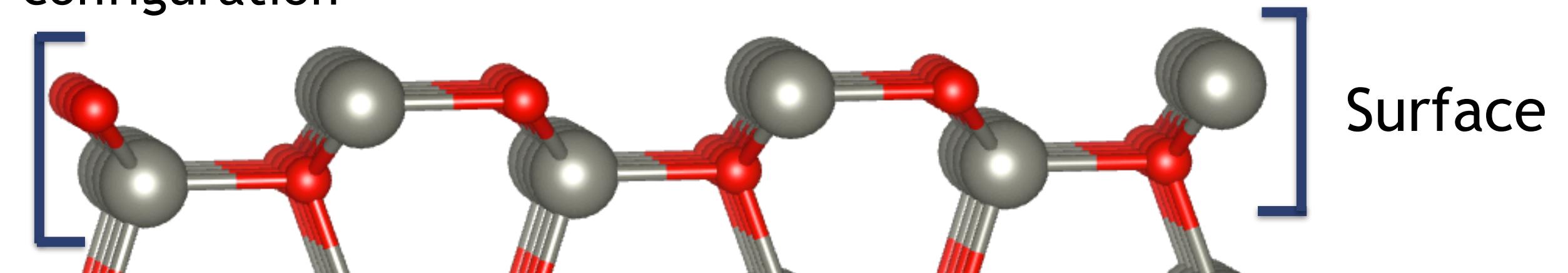


Figure 4: ZnO Surface. This surface is on the side of the nanowire. Oxygen Atoms were removed from that surface layer for the calculations

Table 1: Lattice constant of MgO and ZnO that were confirmed by experimental results seen in Table 2

Material	D{Å}	h k l
ZnO	2.8085	1 0 0
	2.5975	0 0 2
	2.4706	1 0 1
MgO	2.4347	1 1 1
	2.1085	0 0 2
	1.4909	0 2 2

OXYGEN VACANCIES

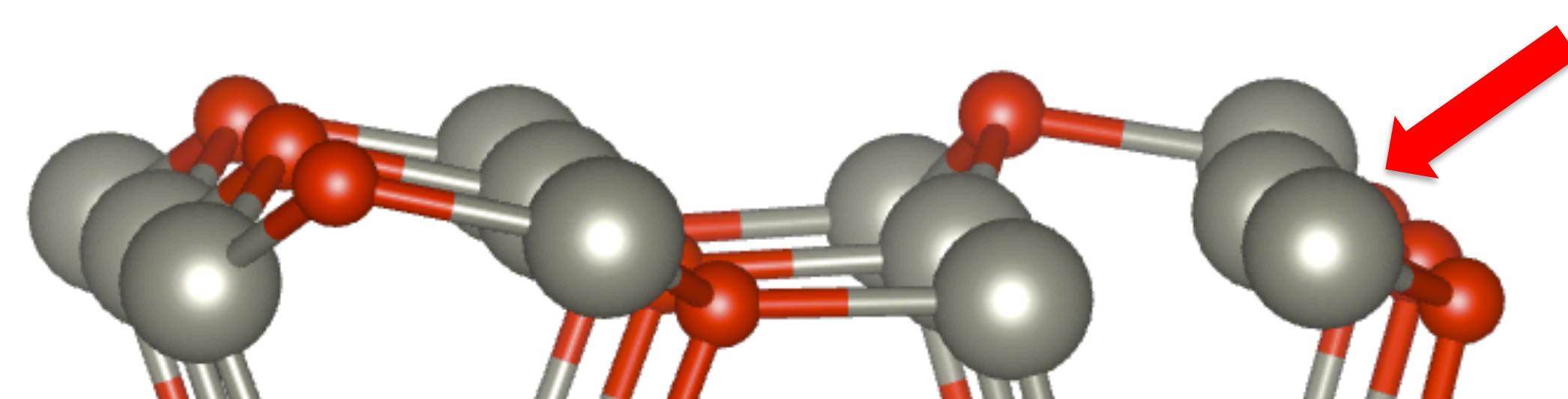


Figure 5: Oxygen vacancies on the surface layer with minor reconstruction indicated by the arrow

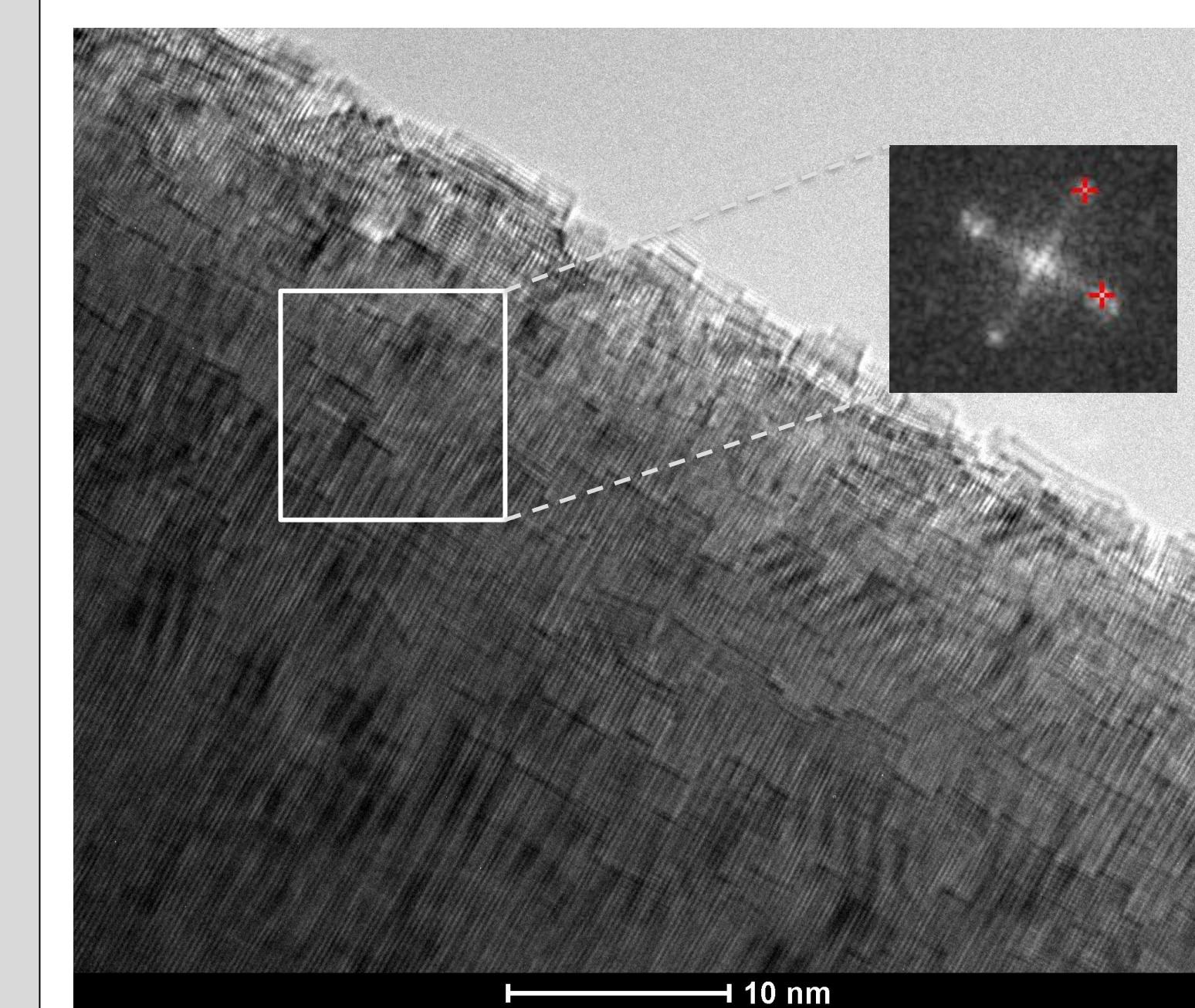
- Oxygen vacancies show no significant ZnO surface reconstruction
- Experiments confirm this conclusion as seen in Figure 5
- Still favorable to MgO wurtzite structure formation

SURFACE ROUGHNESS

- Surface roughness occurred during the growth process

Figure 6: Bare ZnO nanowire surface where the surface roughness can be clearly seen.

RESULTS



Spacing (Å)	h k l	Material
2.62	002	ZnO
2.13	002	MgO

Table 2: Experimental lattice constants in the directions specified, which agree with Table 1

Figure 7: Rocksalt MgO on the surface of ZnO nanowire, that agree with simulation results

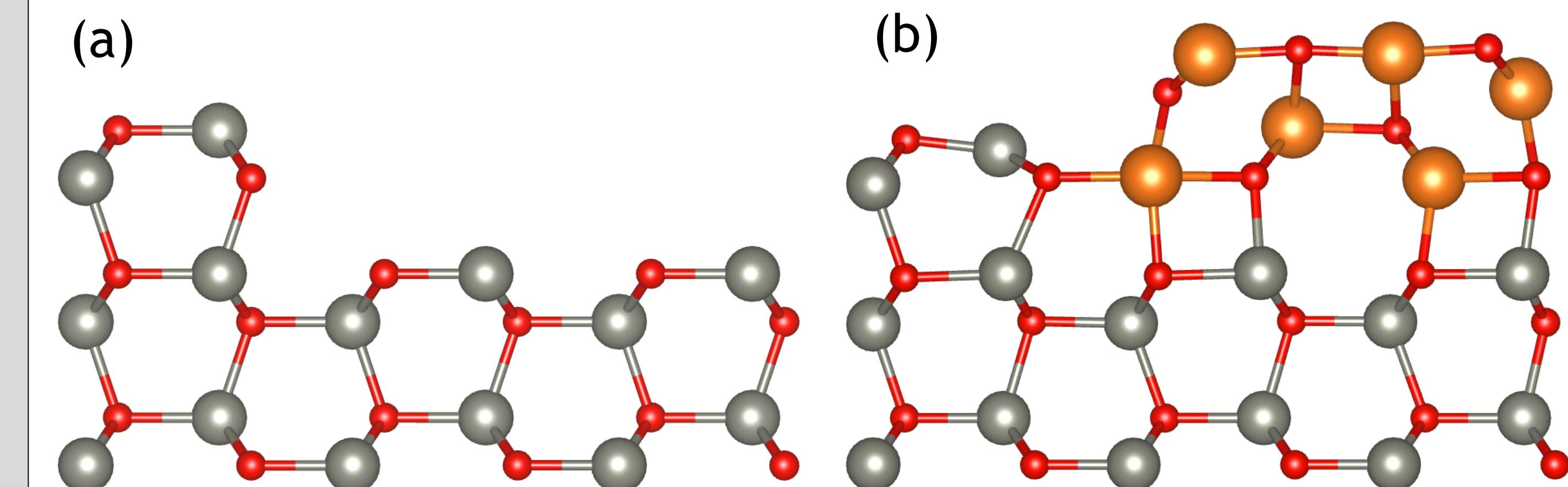


Figure 8: (a) Step in the Surface of ZnO (b) Resulting crystal structure of MgO Rocksalt on the step interface

CONCLUSIONS AND FUTURE WORK

- Oxygen vacancies are not the cause of MgO polycrystalline structure
- Steps on the non-polar ZnO surface are favorable for MgO rocksalt growth
- Steps on ZnO surface and rocksalt growth are seen in experimental data, confirming simulation results

REFERENCES

- D. Mayo, C. Marvinney, E. Bililign, J. McBride, R. Mu, R. Haglund, Thin Solid Films 553 (2014) 132-137
- E. Kaxiras, Atomic and Electronic Structure of Solids

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