氧化物半导体的电子结构部分符合理想热电材料，电性能综合热电性能需要通过掺杂调制，因此项目以形成非平衡态的大失配合金作为手段来可调控性。研究内容瞄准该类材料的形成机理及其微结构/电子结构对热电性能的影响。研究内容包括对大晶格失配合金的理论计算、材料设计、测试平台搭建、脉冲激光沉积工艺下ZnSe/ZnO与ZnTe/ZnO体系不同成分的工艺优化、结构优化及性能研究。从理论计算及实验两个角度表明，O的固溶在ZnSe体系中为置换位缺陷， 其最大固溶量不超过8%左右，同时在O超过4%以上含量时材料的电子结构发生突变，价带中发生明显的轻重带分离，带隙迅速降低到1.8eV左右，经过XPS分析研究发现，Se的部分化学状态处于桥接Zn与O，没有完全形成第二相氧化物沉淀，经过高能脉冲激光沉积及快速退火后处理后，其O析出的程度有所减轻，经过热电性能的测试发现，弱n型材料的输运特征向补偿半导体到重掺杂P型 半导体过渡，热导率同时由于散射增强显著降低，最终ZT值由0.0005上升到0.24;对于ZnTe/.ZnO体系的研究证明，O在其中的位置存在着多种动力学可能位置如Zn缺陷附近形成的团簇体结构以及置换Te形成的置换位结构，这些缺陷结构对能带结构中的中间能带影响较大，同时，PLD工艺本身的刻蚀作用首先使得Te在表面富集，而ZnTe/ZnO体系由于O与Te电负性差异过大然后，O形成TeO2第二相间接导致了Ｏ的固溶量在ZnTe中是ZnSe的一半左右，经过热处理之后，处于多种缺陷态的Ｏ逐渐进入能量更低的置换位缺陷，材料的能带降低到1.68eV左右，最终ZnTe/ZnO体系的p型导电特征加强，热导率降低，ZT值由0.06提高到0.4左右，尽管ZnTe存在着较强的输运特性，但是由于O固溶度相较于ZnSe体系中更低，输运性能的提升程度有限。总而言之，该项目的顺利实施对于研究非平衡态半导体的输运机制，试验提高材料热电性能的设计理念，产生关于大失配氧化物作为一种新型热电材料的理论与实验基础，具有重要的科学意义与应用价值。

The electronic structure of the oxide semiconductor is in accordance with the ideal thermoelectric material. The comprehensive thermoelectric performance of electrical properties needs to be modulated. Therefore, the project uses a large non-equilibrium alloy to form an unbalanced state as a means to regulate and control. The research aims at the formation mechanism of such materials and the influence of their microstructure/electronic structure. The research contents include theoretical calculation of large lattice mismatched alloy, material design, test-platform construction, process optimization, structure optimization and performance research of different components of ZnSe/ZnO and ZnTe /ZnO systems under pulsed laser deposition. From theoretical calculations and experiments, O forms OSedefect in the ZnSe system, and its maximum solubility is lower than 8%, and the electronic structure of the material changes abruptly when O exceeds 4%. Light hole band and heavy hole band separation occurred, and the band gap rapidly decreased to ca. 1.8 eV. It was found that some chemical states of Se are bridging Zn and O, and no second-phase oxide precipitation are formed. After post-annealing by RTA, the degrees of precipitation have been reduced. The transport properties show a behavior of weak n-type materials, and transform to compensating semiconductors and heavily doped P-type semiconductors. The thermal conductivity is decreased due to scattering, and the final ZT value increased from 0.0005 to 0.24. Studies on the ZnTe/ZnO system have shown that there are various possible positions for O, such as the cluster structure formed near the Zn defect and the replacement of Te. These defect structures have a greater impact on the intermediate band in the band structure. At the same time, the etching effect of the PLD enriches Te on surface, the formation of the second phase of TeO2 on the surface directly causes the maximum solubility of O to be about half of ZnSe. After RTA treatment, O gradually enters the displacement defect due to a lower defect formation energy, and the energy band of the material is reduced to about 1.68eV. In the end, the p-type conductivity characteristics of the ZnTe / ZnO system are enhanced, power factors are increased accordingly, and the thermal conductivity is reduced due to phonon scattering. The ZT value is increased from 0.06 to about 0.4. Due to the limited solid solution of O, the degree of improvement of ZT values is only about an order of magnitude.