

Formation of secondary phase particles in compound semiconductor bulk crystals grown from melt

Yadong Xu^{1,2*}, Han Sun¹, Ruicheng Bai¹, Qihao Sun¹, Bao Xiao¹, Mneghua Zhu^{1,2},
Chongjian Zhou,^{1,2} Wanqi Jie^{1,2}

¹Key Laboratory of Radiation Detection Materials and Devices, MIIT

²State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, China

* Email: xyd220@nwpu.edu.cn

The presence of secondary phase (SP) particles significantly affects the optical and electronic properties of the bulk crystals as well as the surface perfection of epitaxial substrates. They appear not only in II-VI (e.g., CdTe, ZnSe), III-V (e.g., GaN), and IV-VI (e.g., SiC) compounds, but also in oxides, halides and fluorides [1, 2]. CdZnTe (CZT) and ZnTe crystals have been studied intensively due to their potential applications in X/γ-ray detection and THz applications. However, localized regions with SP particles (inclusions/precipitates) and induced dislocations are usually generated inevitably in as-grown or post-growth annealed CZT/ ZnTe crystals [3, 4], which are known to be detrimental to the charge collection for CZT detector, simultaneously to degrade the THz emission efficiency of ZnTe electro-optic crystal.

Here, we report the relationship between SP particles and induced dislocations in 2-4 inches CZT/ZnTe bulk crystals. Two possible models for growth and multiplication of dislocation clusters are proposed on the basis of dissociation-diffusion and thermomigration-deformation, respectively. Then, we developed an improved annealing method, which the annealing temperatures are optimized during one annealing cycle to reduce or even eliminate the SP particles. In addition, the formation of SP particles in the centimeter-size typical chalcogenide semiconductor and metal halide perovskite crystals is also revealed.

References:

- [1] Peter Rudolph, Dislocation patterning and bunching in crystals and epitaxial layers-a review, *Crystal Research and Technology*, 2017, 52: 1600171.
- [1] Yuanbo Cheng, Qihao Sun, Peng Zhang, et al., Secondary Phase Particles in Cesium Lead Bromide Perovskite Crystals: An Insight into the Formation of Matrix-Controlled Inclusion. *Journal of Physical Chemistry Letters*, 2020, 11, 5625-5631
- [3] Yihui He, Wanqi Jie, Yadong Xu, et al., Matrix-controlled morphology evolution of Te inclusions in CdZnTe single crystal. *Scripta Materialia*, 2012. 67(1): 5-8.
- [4] Zihan Wei, Yadong Xu*, Bao Xiao, et al., Homogenization of Te-rich grown ZnTe bulk crystals by annealing under Zn vapor. *CrystEngComm*, 2019, 21(2): 283-289.

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