

# Study on growth and doping of large scale gallium selenide crystals

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Gallium selenide (GaSe) crystal is a mid-range infrared nonlinear optical material with excellent performance, and has a wide transmission range and a less low absorption coefficient [1]. However, the crystal has a low hardness and easily dissociated along the c axis [2]. By doped S and In elements, to compensate the defects. In this paper, GaSe and doped polycrystalline materials were synthesized by two-temperature method, and GaSe and doped single crystals were grown by vertical Bridgman method. The theory of first principles is applied to theoretical study of crystals.

We successfully produced a 40 mm diameter GaSe single crystal. XRD characterization showed that the crystal grown along the (004) plane. The transmission range of GaSe was measured by infrared spectroscopy to be 0.65  $\mu\text{m}$  -20  $\mu\text{m}$ , and the transmittance was stabilized at 65%. The rocking curve test results show the half-peak width is 47.76", and the single crystal is better. Scanning electron microscopy shows that there are defects such as vacancies and inclusions in the crystal monolayer. The nano-hardness and the elastic modulus of GaSe tested by nanoindentation hardness tester are 0.94 GPa and 27.3 GPa, respectively.

GaSe<sub>1-x</sub>S<sub>x</sub> (x = 0.008, 0.1, 0.2) single crystal was successfully grown. XRD characterization shows that the S-doped single crystal grown at a low concentration is still growing along the (004) plane. The transmission range of GaSe<sub>0.8</sub>S<sub>0.2</sub> was extended to 0.59  $\mu\text{m}$ -20  $\mu\text{m}$  by infrared spectroscopy. GaSe<sub>0.9</sub>S<sub>0.1</sub> had the best effect, the transmittance was 65.3%, and the half-peak width was 53.61", the nanohardness is 1.34 GPa, and the elastic modulus is 28.8 GPa. Theoretical calculation shows that the band gap value increases after doping S element, the degree of internal anisotropy decreases, the refractive index, reflectance and absorption rate are reduced.

Single crystal of Ga<sub>1-x</sub>In<sub>x</sub>Se (x=0.003, 0.007, 0.013) was successfully grown. XRD characterization shows that doped with In is still growing along the (004) plane. The effect of Ga<sub>0.993</sub>In<sub>0.007</sub>Se was the best effect in the In concentration, and the transmittance was stable at 65.2%. The half-peak width is 53.61", the nanohardness is 1.03 GPa, and the elastic modulus is 28.5 GPa. Theoretical calculation shows that the band gap value of the doped In element crystal is basically unchanged, and the degree of anisotropy inside the crystal increases. The refractive index, reflectance, and absorptivity all reduced.

## References

- [1] Zhu CQ et al. Synthesis and growth of GaSe single crystals. J Cryst Growth. 2015;421:53-57.
- [2] Abdullah MM et al. Growth and characterization of GaSe single crystal. J Cryst Growth. 2010;312:1534-1537.