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A first step towards Understanding CZTS $\Sigma 3$ (112) family grain boundaries MAN HOI WONG, KIN FAI TSE, JUNYI ZHU, Chinese University of Hong Kong — CZTS is a promising low cost, earth abundant solar cell absorber material for thin film solar cell. Grain boundary properties are crucial in the performance enhancement of the solar cell device, yet not well studied. This work is dedicated to the characterisation of $\Sigma 3$ grain boundaries with and interfaces, which are also found to be abundant experimentally. DFT calculations with GGA exchange functional is used to calculate the structure of those grain boundaries. Using modified wedge method, formation energies of different reconstructed grain boundary and relevant surfaces were calculated from various slabs. According to our calculations, we found a repulsive grain boundary based on anion-anion terminations with low formation energy. Such problematic grain boundaries may widely distributed in the device and hinder the performance. In addition to the structure studies, Electronic structures of low energy grain boundaries were calculated to understand their impact on device efficiency. Our results match very well with observations from previous experimental works. It provided a solid foundation for future studies of grain boundary engineering, which could be crucial to the success of CZTS.

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