Self-passivation Rule and the Effect of Post-treatment in GBs of Solar Cell Materials

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Abstract

Grain boundaries (GBs) existing in polycrystalline semiconductors alloys inducing a great deal of deep defect levels are usually harmful to cells' photovoltaic performance. Experimental and theoretical investigations verified that these defect levels come from the GBs' dangling bonds. We find that, the defect levels in anion core of GB can be passivated by its cations, called by self-passivation. For instance, the post-treated by $CdCl_2$, Cd can eliminate the defect levels by saturating Te dangling bonds in the grain boundary of CdTe. We verify that the idea of self-passivation rule can perfectly explain the benign GBs of CISe and CZTS by sodium treatment. The present work reveals a general mechanism about how dopants in GBs eliminate the defect states through passivating the dangling bonds in covalent polycrystalline semiconductors, and sheds light on how to passivate dangling bonds in GBs with alterative processes.

References

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