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Epitaxial growth of CuInSe₂/InSe/Si heterostructures for photovoltaic applications

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Next generation Si solar cell is heading for the use of ultra-thin Si wafers with the thickness less than 50 μ m. The challenge is to develop an effective light trapping technology for the PV cells in this category since crystalline Si is an indirect-gap material with a low optical absorption coefficient. In this work, we develop a novel device structure using an efficient light absorption layer of CuInSe₂ (CIS) at the bottom of Si homojunction. The device under investigation possesses epitaxial structure on single-crystalline Si substrate. Since the lattice mismatch of CIS/Si is considerable large, the insertion of a thin layer of 2D compound (InSe) at the interface is employed to solve the mismatch problem (so-called van der Waals epitaxy). Device simulation using PC1D indicates that the cell efficiency of a device structure of n-Si/p-Si/InSe/p-CIS may reach 32.5% under AM 1.5 illumination as the wafer thickness down to 5 μ m. An additional role of InSe is to create a band alignment which is favorable to separate the electron-hole pairs produced in CIS and transport in opposite directions. It is more like a tandem-cell structure so that a decent energy conversion efficiency can be achieved. The simulation has considered the interface recombination and used the up-to-date material parameters reported in the literature. To verify the simulation results, a molecular beam epitaxy (MBE) technique is employed to grown an interfacial layer of InSe on (100)Si prior to the deposition of a CIS film. With the use of a Hg lamp to conduct the photo-assisted growth, we are able to grow epitaxial CIS films at a temperature as low as 300oC. This temperature prohibits the interdiffusion in the heterostructure as confirmed by our TEM microanalysis. The fabrication and properties of the above-mentioned device structure will also be reported in the conference.

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