Defect states at c-Si/a-SiN:H interfaces

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Computational Materials Physics

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Modern electronic devices are unthinkable without the controlled formation of interfaces at heterostructures. These often involve at least one amorphous material. Modeling such interfaces poses a significant challenge, since a meaningful result can only be expected by using huge models or by drawing from many statistically independent samples. Here we report on the results of high throughput calculations for interfaces between crystalline silicon (c-Si) and amorphous silicon nitride (a-Si3N3.5:H), which are omnipresent in commercially available solar cells. The findings reconcile many hardly understood key features. At the interface, many threefold coordinated Si atoms are present. These are caused by the structural mismatch between the amorphous and crystalline part. The local Fermi level of undoped c-Si lies well below that of a-SiN:H. To align the Fermi levels in the device, charge is transferred from the a-SiN:H part to the c-Si part resulting in an abundance of positively charged, threefold coordinated Si atoms. This explains the existence of a positive, fixed charge at the interface that repels holes.