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Infrared absorption enhancement at nickel-silicide/silicon interfaces JORDAN HACHTEL, ROHAN MISHRA, SOKRATES PANTELIDES, Vanderbilt Univ., Oak Ridge National Laboratory, STEPHEN PENNYCOOK, Oak Ridge National Laboratory — Nanoparticle embedded thin films are of interest because they have been predicted to enhance absorption and improve thin-film photovoltaic devices. For the case of nickel silicide nanoparticles embedded in amorphous silicon there is experimental observation of absorption enhancement, especially in the infrared where the solar spectrum is strong, but silicon absorption is weak. However, it is not known whether this enhancement is due to effects at the silicide/silicon interface that can actually be applied to photovoltaic devices or simply bulk absorption into the metal. To study these effects, we created theoretical supercells of the interface between nickel di-silicide and silicon, and calculate the optical properties using density functional theory. The supercells show a strong absorption enhancement peak in the red/near-IR, which is the optimal region for absorption. An analysis of the DOS reveals that shifts in the dominant nickel d-orbitals create interface transitions in the IR that are unavailable in the bulk.

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