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Electrical and optical properties of PtSi thin films HENDRIK BENTMANN, A.A. DEMKOV, UT Austin, STEFAN ZOLLNER, RICH GREGORY, Freescale Semiconductor — Metal silicides are used in complementary metal-oxide-semiconductor devices (CMOS) to form contacts between metal interconnects and source, drain, and gate silicon of the transistors. They offer important properties like low resistivity, low contact resistance to Si as well as excellent process compatibility with the standard Si technology. Recently, metal silicides have attracted renewed attention and they are a current research topic in the semiconductor industry. We report a joint theoretical and experimental study of thin Pt silicide films. Employing density functional theory (DFT) methods we have investigated the electronic structure as well as bonding and optical properties of PtSi and Pt_2Si. Additionally, we have calculated surface energies for various orientations and terminations of PtSi surfaces. Our results suggest that thermodynamics plays an important role in the silicide formation. The complex index of refraction determined by spectroscopic ellipsometry exhibits non-Drude behavior and shows peaks, which were identified with inter-band transitions in the d-manifold of platinum and compared to theory.

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