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Surface States and rectification at a Metal high-k Dielectric Contact ALEX DEMKOV, Freescale Semiconductor, Inc. — The properties of metal-to-insulator junctions are often discussed in terms of the Fermi level pinning by the interface states. An alternative point of view is based on the picture of polarized chemical bonds at the metal-to-insulator interface. We consider theoretically the case of molybdenum on the (111) surface of the tetragonal polymorph of hafnia, and trace the formation of the Schottky barrier from the Newens-Anderson chemisorption limit to a one nm thick layer of the (110) oriented metal. The role of the surface band of hafnia in the pinning of the Fermi level is discussed, including the analysis of relative roles of the evanescent and chemical interface states. We critically compare the predictions of the metal induced gaps states (MIGS) model with the results of direct density functional calculations.

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