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Current Schottky Barrier Concepts

RAYMOND TUNG, Department of Physics, Brooklyn College, City University of New York

The formation of Schottky barrier height at metal- semiconductor interfaces has been a subject of intense investigation and heated debate for over three decades. Early studies largely concentrated on the explanation of the experimentally observed “Fermi level pinning” phenomenon, the apparent lack of a strong dependence of the barrier height on the metal work function. Theories proposed early on typically relied on some empirical assumptions/mechanisms to explain the weak dependence of the barrier height on the metal, the most notable of which was the assumption that the distribution of the interface states was independent of the metal. This assumption has subsequently been shown by numerous ab initio calculations to be without basis. Experimental results contrary to the notion of “pinning” were also observed. For example, on well-controlled interfaces a sharp dependence of the barrier height on the interface atomic structure was experimentally established, as was a pervasive inhomogeneity of barrier height at polycrystalline interfaces. Recently, a simple analysis, by molecular chemical methods, reveals that the dipoles from bond polarization are in excellent agreement with the observed strength of the Fermi level pinning on different semiconductors. A host of seemingly contradictory experimental observations in the field of Schottky barrier heights thus seems reconcilable within one coherent explanation. In this presentation, a brief account of Schottky concepts, both old and new, will be given. The basis for the recent theoretical chemical analysis, as originally intended for molecular studies, and the steps that were taken for application to solid metal-semiconductor interfaces will be examined. Also will be discussed are further modifications of this scheme for applications to other material interfaces of current interest, such as the energy level alignment at organic interfaces and the band offsets at oxide interfaces. A particular emphasis is placed on the consistency that should be achieved between the condition assumed for the components of the interface and the method adopted to estimate the charge transfer. For the latter, a brief examination of existing concepts of group electronegativity will also be given.