Quantum Mechanical Calculations of Electromigration Characteristics

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Since electromigration has been for the first time observed and initial theoretical and semi-empirical models have been developed, an extraordinary importance of one parameter has been recognized: the effective valence. The effective valence characterizes the susceptibility of the interconnect metal to electromigration and establishes a linear relationship between the electromigration force and an external electric field. Very early in the history of electromigration studies, experimental methods have been developed, which enable the experimental determination of the effective valence for a wide spectrum of metals. These methods, even if they have provided reliable values of the effective valence, did not provide a deeper insight in the true origin and the nature of the electromigration phenomena. Moreover, values for the effective valence could have been obtained only for the bulk regions of a metal, while at the same time technologically-related research has pointed out the importance of electromigration in metallic grain boundaries, interfaces, and surfaces. Starting with the semiclassical ballistic electromigration model presented in the pioneering work of Huntington, the quantum mechanical nature of the electromigration phenomena has been gradually understood. I will present an overview of the main electromigration quantum mechanical models developed since the 1970s and the corresponding numerical approaches for a calculation of the electromigration force and the effective valence. Particular emphasis will be put on the work of Sorbello and the successive efforts together with their foundations in the work of Feynman and Kubo's linear-response theory. Electromigration on the quantum mechanical level is an electron scattering process and, thus, at the heart of any numerical method for calculation of the effective valence stands the determination of the electron scattering states and the electron density. In connection to the problem of scattering states in electromigration theory, methods for determination of electronic structures, like the augmented-plane-wave method and the pseudopotential method will be explained. Finally, some major results about the quantum mechanical nature of electromigration and calculations of the effective valence will be presented.