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Field Emission Mechanisms of Covalently Bonded Nanostructures MASAOKI ARAIDAI, Tokyo University of Science, CREST-JST, KAZUYUKI WATANABE, Tokyo University of Science, CREST-JST — Carbon materials have been found in various forms depending on the different covalent bondings, and intensively studied in anticipation of their application to new nanometer-scale devices. Among the various applications of these covalently bonded nanostructures, electron field emitters made from carbon materials show significant promise for electronic devices, because they can maintain stable forms under extremely high field-emission (FE) current densities owing to tight covalent bonds. In this study, FE mechanisms and the electronic-states origin of covalently bonded nanostructures are microscopically investigated by first-principles calculations based on time-dependent density-functional theory. First, we investigate the FE of silicon clusters and extract a theoretical basis for understanding covalently bonded field emitters. Second, calculations of the FE of diamond C(100) surfaces are carried out and effects of hydrogen terminations and hydrogen defects in the subsurface on the FE are discussed by using electronic band structures. Finally, we address the effects of the electric-field direction on the FE characteristics of graphenes and graphitic ribbons. Central results in our study are that not only evaluation of work functions but also knowledge of local electronic properties, the σ - or π -bonding states, are prerequisite for understanding the microscopic mechanisms of FE properties of covalently bonded nanostructures.

Masaaki Araidai
Tokyo University of Science, CREST-JST

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