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Schottky junctions studied using Korringa–Kohn-Rostoker nonequilibrium Greens function method[1] HISAZUMI AKAI, Univ of Tokyo, MASAKO OGURA, Department of Chemistry, University of Munich and Department of Physics, Osaka University — A scheme that combines the non-equilibrium Greens function method with the Korringa–Kohn–Rostoker (KKR) Greens function method is proposed. The method is different from many previous attempts in that it uses the exact Greens function whose spectrum is not bound within a finite energy range, and hence, provides sound basis for quantitative discussions. The scheme is applied to the Schottky junctions composed of an Al/GaN/Al trilayer. Schottky contacts formed in metal/semiconductor junctions play an important role in semiconductor devices and integrated circuits. They have been intensively investigated for several decades not only for possible application to electronic devices but also for gaining a fundamental understanding of the Schottky barrier formation. Our results show that the Schottly barrier is formed between an undoped GaN and Al interface. The transport property of this system under various finite bias voltages is calculated. It is shown that the asymmetric behavior of electron transport against the direction of bias voltage occurs in this system, confirming the feature of rectification.

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