Non-equilibrium Low-Energy Transport Physics of Electron and Phonon at Nanoscale

Y. Asai
Nanosystem Research Institute (NRI) "RICS,"
National Institute of Advanced Industrial Science and Technology (AIST),
Umezono 1-1-1, Tsukuba Central 2, Tsukuba, Ibaraki 305-8568, Japan
e-mail: yo-asai@aist.go.jp

INTRODUCTION

Because electronic devices become smaller than before they were, first principle based non-equilibrium transport theory becomes applicable to some of the important devices in nanoelectronics nowadays. One of the examples is the resistive random access memories (ReRAMs) whose device length scale becomes smaller than 10 nano meter (nm) [1]. First principle transport theory, however, has some intrinsic limitations. Because it is based on a ballistic transport theory, it cannot take into account of scattering effects, heating effects, heat dissipation effects and the hopping conduction processes. All of these, however, have been a matter of intense investigations among condensed matter physics theorists. A theory describing all of these has been developed recently. In this talk of 16th IWCE, I will describe the present status of the theory in this respect.

THEORY

Because paramagnetic electronic correlation effect is mostly elastic, the largest contribution to the heating effects may come from electron-phonon interactions. [2] The interaction effects on electric current *I* are described by the following equation:

$$I = \frac{2e}{h}\int Tr[\Sigma_L^{>}(E)G_R^{<}(E) - \Sigma_L^{<}(E)G_R^{>}(E)]dE + \frac{2e}{h}\int Tr\left[\Sigma_L^{>}(E)G_{eph}^{<}(E) - \Sigma_L^{<}(E)G_{eph}^{>}(E)\right]dE$$

where $G_{eph}^{<(>)}(E) = G^R(E)\Sigma_{eph}^{<(>)}(E)G^A(E)$ and $G_R^{<(>)}(E) = G^R(E)\Sigma_R^{<(>)}(E)G^A(E)$.

$\Sigma_{eph}^{<(>)}$ is the Keldysh component of the electron-phonon self-energy, which may be obtained by using the self-consistent Born approximation (SCBA) for example. $\Sigma_R^{<(>)}$ is the contact self-energy of the right terminal which is obtained by using surface electron Green's function of the right electrode terminal and the thermal equilibrium boundary condition. Electrode terminals are supposed to be thermalized and all the heat generetated by the electron-phonon interaction is supposed to be dissipated there. In order to take into account of the heat dissipation effect on the curret *I*, we take into account of phonon current as well as electron current whose schemes werer discussed in the reference [3].

APPLICATIONS

The theory [3] has been tested in some cases of single molecular junctions which are made of a single molecule and two bulk electrodes. Break junction techniques are applied to them and statistical analyses of the resulting data are made. Acurate experimental results comparable with the theory are thus obtained. The local heating effect [4,5], the cross over temperature dependence of the conductance describing both the tunneling and the hopping regions [6] and the zero bias anomaly (ZBA) of electric conductance [7] have been discussed. Good agreements between the theoretical and experimental results affirm the validity of the theory to describe low-energy

978-3-901578-26-7

transport physics and thermal physics of electron and phonon. [5-9]

RESULTS

The local heating effect result and the ZBA result are summarized in Figs. 1 and 2, respectively. As we apply the bias voltage *V*, the effective temperature T_{eff} defined in terms of the break junction life time [5,8,9] increases with small deviation from the estimate obtained by using bulk phonon theory, i.e., $T_{eff}^4 \propto V^2$. The deviation may come from the constriction effect on phonon current. In Fig.2, the ZBA behavior emerging in the inelastic tunneling spectrum (IETS: d^2I/dV^2 vs *V* spectrum) is shown. While the growth of peak and dip structures at positive and negative values on the voltage axis whose absolute value correspond to phonon energy is the well-known feature of the IETS, the growth of a structure close to *V=0* is quite anomalous. This zero bias anomaly has been observed experimentally. Our theoretical results indicate that the ZBA comes from rattling motion of the molecule in the gap between the two electrodes. Our theory is capable to describe the low energy transport physics of our junction.

CONCLUSION

By including phonon transport as well as electron transport, our theory treating electron-phonon interaction within the SCBA can describe low energy transport physics and thermal physics problems including heat dissipation into the thermalized electrodes. Our theory should be very useful when it is applied to nanoelectronics problems.

REFERENCES

[1] T. Miyazaki, H. Nakamura, K. Nishio, H. Shima, H. Akinaga, and Y. Asai, unpublished results.

[2] Y. Asai, *Theory of inelastic electric current through single molecule,* **Phys. Rev. Lett**. 93, 246102-1-4 (2004).

[3] Y. Asai, *Nonequilibrium phonon effects on transport properties through atomic and molecular bridge junctions,* **Phys. Rev. B** 78, 045434-1-24 (2008).

[4] Y. Asai, H. Nakamura, J. Hihath, C. Bruot, and N.J. Tao, *Electron correlation enhancement of the diode property of asymmetric molecules,* **Phys. Rev. B** 84, 115436-1-5 (2011).

[5] Y. Asai, *Theory of local heating in single molecular bridge junctions,* **Phys. Rev. B**, 84, 085436-1-7 (2011).

[6] S. –K. Lee, R. Yamada, S. Tanaka, G. –S. Chang, Y. Asai, and H. Tada, *Universal Temperature Crossover Behavior of Electrical Conductance in a Single Oligothiophene Molecular Wire,* **ACS Nano**, 6, 5078-5082 (2012).

[7] Y. Asai, *Theory of zero-bias anomaly in low-temperature inelastic tunneling spectroscopy*, **Phys. Rev. B** 86, 201405(R)-1-4 (2012): Rapid Communications.

[8] Z. Huang, B. Xu, Y. Chen, M. Di Ventra, and N.J. Tao, *Measurement of Current-Induced Local Heating in a Single Molecule Junction,* **Nano Lett**. 6, 1240 (2006).

[9] Z. Huang, F. Chen, R. D'Agosta, P. A. Bennett, M. Di Ventra, and N.J. Tao, *Local ionic and electron heating in single-molecule junctions*, **Nature Nanotech**. 2, 698 (2007).

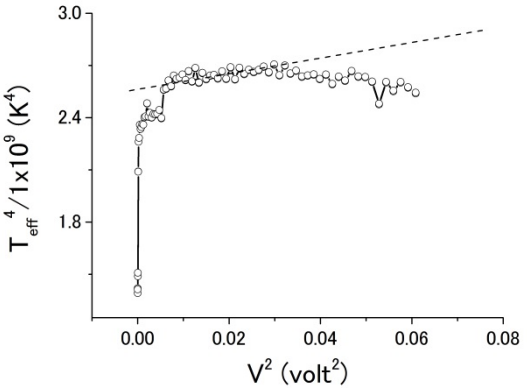

Fig. 1. The voltage dependence of the effective temperature T_{eff} estimated from the junction lifetime. The result agrees with experimental results qualitatively.

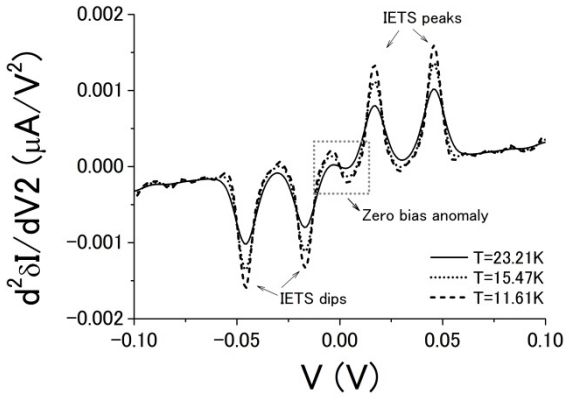

Fig. 2. The zero bias anomaly found in the IETS. The similar anomaly has been found experimentally.