Physics Letters A 380 (2016) 942–950

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Magnetoresistance effect of heat generation in a single-molecular spin-valve

Feng Jiang [a,*], Yonghong Yan [b,*], Shikuan Wang [c], Yijing Yan [d,e]

[a] School of Mathematics and Physics, Shanghai University of Electric Power, Shanghai, 200090, China
[b] Department of Physics, Shaoxing University, Shaoxing 312000, China
[c] Department of Physics, Hangzhou Dianzi University, Hangzhou 310018, China
[d] Department of Chemistry, Hong Kong University of Science and Technology, Kowloon, Hong Kong, China
[e] Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China

ARTICLE INFO

Article history:
Received 10 October 2015
Received in revised form 16 December 2015
Accepted 23 December 2015
Available online 30 December 2015
Communicated by R. Wu

Keywords:
Heat generation
Spin-valve
HMR
TMR
e–ph
e–e

ABSTRACT

Based on non-equilibrium Green's functions' theory and small polaron transformation's technology, we study the heat generation by current through a single-molecular spin-valve. Numerical results indicate that the variation of spin polarization degree can change heat generation effectively, the spin-valve effect happens not only in electrical current but also in heat generation when Coulomb repulsion in quantum dot is smaller than phonon frequency and interestingly, when Coulomb repulsion is larger than phonon frequency, the inverse spin-valve effect appears by sweeping gate voltage and is enlarged with bias increasing. The inverse spin-valve effect will induce the unique heat magnetoresistance effect, which can be modulated from heat-resistance to heat-gain by gate voltage easily.

1. Introduction

In the past thirty years, with the development of micromachining technology, semiconducting electronics have made enormous progress. According to the latest progress, the size of the electron devices has reached about 20 nm in mainstream CPU, and its operation frequency has reached several GHz. With these advancements, one critical issue, i.e., the heat generation from electric currents has emerged. The large amount of accumulated heat caused by the current makes the chip's temperature rise to a such high level that the chip may not work properly. This dissipation in nanodevices strongly hinders further development of the semiconductor electronics. Usually there are two ways to reduce the chip's temperature: one is to remove the heat as quickly as possible, the other is to suppress the heat generation. But the complex device geometries normally make heat removal very difficult with the improving of integration level. Thus, it is very important to discover the laws of heat generation induced by electric currents in nanodevices and to investigate how the heat generation may be reduced.

From a microscopic point of view, the main heat generation is due to electron–phonon interactions, through which the energy associated with the electric current in an electronic system is transferred to the phonon system in the form of heat [1]. The heat generation in macroscopic systems, the Joule effect is well known and similar studies in nanodevices, that only began a few yeas ago, have made some gratifying progress. On the experimental side, the variance of local temperature in a nanoscale junction due to the bias voltage has been observed [2]. On the theoretical side, using non-equilibrium Green's function (NEGF) [3], a general formula for the current-induced heat generation was derived by Sun's group [4]. The investigation of current-induced local heating in nanodevices has found the unique relation between heat generation and charge current which is different from the Joule effect in macrodevices [4–10].

However, most previous works focus on the spin non-polarized devices and the heat generation in spin-polarized devices has not been studied seriously so far, while due to advances in materials science and nanofabrication techniques, spintronics has become more and more attractive and exciting [11]. In spintronics, one interesting and important effect for spin-polarized transport is the tunneling

---

[*] Corresponding authors.
E-mail addresses: fjiang@shiep.edu.cn (F. Jiang), yhyan@fudan.edu.cn (Y. Yan).

http://dx.doi.org/10.1016/j.physleta.2015.12.025

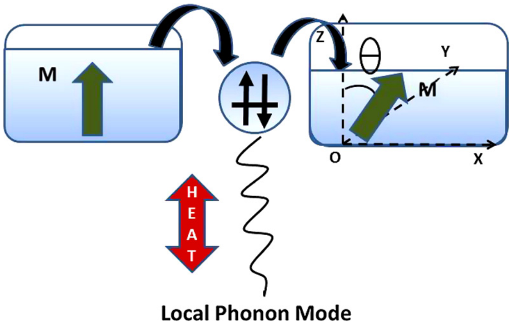

Fig. 1. Schematic plot showing the TMR device based on a single MQD coupled with two FM leads and a local phonon mode.

magnetoresistance (TMR) [12]. A TMR device is usually presented by combinations of an insulating (I) material layer sandwiched in between two ferromagnetic (FM) layers, forming an FM/I/FM tunneling structure. TMR devices have also shown sensitive magnetoresistance behavior at room temperature, and one of the particular attractions of a TMR device is that it carries lower current than the metallic giant magnetoresistance (GMR) [13] system which is a helpful device characteristic.

The simplest TMR device is a molecular junction consisting of a molecular quantum dot (MQD) coupled through tunnel barriers to FM leads [14,15]. In the molecular junction two types of important interactions have a great influence on the electron tunneling through the MQD, one is electron–electron (e–e) interaction, the other is the electron–phonon (e–ph) interaction due to vibrational degrees of freedom in the MQD. The e–e interaction will result in Coulomb blockade and the e–ph interaction will induce the I–V staircase [16–19]. The extensive studies show many unique transport characteristics of the F/MQD/F junction, for example, e–ph coupling results in the oscillation of TMR [14,20]. But for the strong operability, as the representative of spin-polarized devices, its heat generation characteristics are to be discovered. Now one key question should be answered, that is how the heat generation changes with the variation of the electrodes' polarization and how to understand and utilize these heat-behaviors.

In this paper, we use NEGF combined with small polaron transformation to study heat generation by current through a single-molecular spin-valve and find the spin-valve and spin-polarization degree can modulate heat generation effectively and the interesting inverse spin-valve effect is found by increasing bias. In addition, we also find both heat-resistance and heat-gain can be achieved easily by gate voltage and bias. The paper is organized as follows. In Section 2, the model Hamiltonian gives the general descriptions for an open MQD coupled with one local phonon mode and two FM leads and the small polaron transformation of the Hamiltonian is also shown. In Section 3, the formula of current and heat generation for FM leads is derived. In Section 4, the numerical calculations and discussions are presented. Finally, we give our concluding remarks in Section 5. In Appendix A, the retarded Green's function is solved by the technology of equations of motion in detail.

2. The model Hamiltonian and small polaron transformation

The general device structure we consider is schematically shown in Fig. 1, where a single MQD is coupled to two FM leads. Inside the MQD there are e–e and e–ph interactions. The permanent magnetic moments of the leads are denoted by the vector $\mathbf{M}_\alpha$, where $\alpha = L, R$ indicates the left and right leads. The general hamiltonian is expressed as follows [21]:

$$
\begin{aligned}
H &= H_{\text{ph}} + H_{\text{e-ph}} + H_{\text{e}},\\
H_{\text{ph}} &= \omega_0 \hat{b}_0^\dagger \hat{b}_0,\\
H_{\text{e-ph}} &= \lambda(\hat{b}_0^\dagger + \hat{b}_0)\sum_\sigma \hat{n}_{d\sigma},\\
H_{\text{e}} &= \varepsilon_0(t)\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{\alpha k\sigma}[\epsilon_{\alpha k}(t) + \sigma M_\alpha]\hat{n}_{\alpha k\sigma}\\
&\quad + \sum_{\alpha k\sigma}[t_{\alpha kd}(\cos\frac{\theta_\alpha}{2}\hat{a}^\dagger_{\alpha k\sigma} - \sigma\sin\frac{\theta_\alpha}{2}\hat{a}^\dagger_{\alpha k\bar{\sigma}})e^{i\sigma\phi_\alpha/2}\hat{d}_\sigma + \text{H.c.}],
\end{aligned}
\tag{1}
$$

where, λ is the e–ph coupling constant and $\hat{b}_0^\dagger$ ($\hat{b}_0$) is the creation (annihilation) operator for the located optical-phonon mode of the MQD with the vibration frequency ω_0, $\varepsilon_0(t)$ is a spin-degenerate, and time-dependent level in the MQD and $\hat{d}_\sigma^\dagger$ ($\hat{d}_\sigma$) is the creation (annihilation) operator of the electron level with spin σ in the MQD, $\hat{n}_{d\sigma}$ is the corresponding spin-dependent particle-number operator, U denotes the intradot Hubbard interaction between electrons with the reverse spin, $\epsilon_{\alpha k}(t)$ is a spin-degenerate and time-dependent level in the α-lead, M_α as a magnetic moment shows the difference of density of states (DOS) between spin-up and spin-down electrons in the α-electrodes and $\sigma = \pm 1$ for spin-up (spin-down), $\hat{a}^\dagger_{k\alpha\sigma}$ ($\hat{a}_{k\alpha\sigma}$) is the creation (annihilation) operator of the k_{th} level with spin σ in the α-lead, and $\hat{n}_{\alpha k\sigma}$ is the corresponding spin-dependent particle-number operator, $t_{\alpha kd}$ is spin-independent tunneling matrix element between the α-electrode and the MQD.

Note that the spin-up directions in the left FM lead, the MQD, and the right FM lead are all different, although they are all aligned in their local z directions. In the MQD, the spin-up direction is still in the original z axis, but in the left and right FM leads, the spin-up direction is aligned with the FM moment $\mathbf{M}_{L/R}$. For simplicity, the magnetic moment is assumed to be a constant value in each lead and $|\mathbf{M}_L| = |\mathbf{M}_R| = |\mathbf{M}| = M$, $\mathbf{M}_L$ is pointing to the z direction, while $\mathbf{M}_R$ is at an angle θ to the z axis in the x–z plane. (For the simplicity