Kondo-Fano resonance in atomic-scale contacts for ferromagnetic metals

MS Islam[1], H Takata[1], Y Ueno[1], K Ienaga[2], Y Inagaki[1], H Tsujii[3] and T Kawae[1]

[1]Department of Applied Quantum Physics, Kyushu University, Fukuoka, Japan

[2]Department of Physics, Tokyo Institute of Technology, Tokyo, Japan

[3]Division of Science Education, Kanazawa University, Kanazawa, Japan

E-mail: sislamru@gmail.com

Abstract. The electrical conductance of cobalt (Co) nano-scale contacts prepared by a Mechanically Controllable Break Junction (MCBJ) technique has been studied to understand the origin of Fano resonance in ferromagnetic atomic-sized contacts. In an atomic-scale contacts, the zero-bias anomaly is well-fitted by the Fano formula. The characteristic temperature, which is introduced as the fitting parameter of that formula, exhibits the log-normal distribution. These indicate that the anomaly is likely caused by Kondo effect. Moreover, the zero-bias anomaly is observed in large scale contacts where the bulk ferromagnetic properties should be retained. This suggests the coexistence of Kondo effect and ferromagnetism.

Keywords: Kondo effect, Fano resonance, MCBJ, Electrical properties

1. Introduction

The Kondo effect is understood as the quenching of a magnetic impurity by the bath of conduction electrons and forming a singlet ground state [1] and is observed in a variety of systems ranging from bulk magnetic materials to nanosystems such as single magnetic adatoms on nonmagnetic surfaces, quantum dots, single-electron and -molecule transistors [2-7]. In nanosystems, the Kondo resonance has been observed directly through the Fano anomalies using spectroscopy measurements [8].

During the last few decades, a lot of sustainable effort has been devoted to form and analyze atomic-sized contacts in $3d$ ferromagnetic materials theoretically and experimentally to study the magnetoresistance at the domain wall in nano-sized constrictions. Calvo *et al*. first recorded a zero-bias anomaly in atomic-scale contacts of ferromagnets such as Fe, Co and Ni prepared by scanning tunneling microscopy (STM) and electromigration technique. It is surprising that the anomaly is well-reproduced by the Fano resonance and the amplitude shows logarithmic temperature dependence because these suggest that the anomaly is caused by the Kondo resonance [9]. In addition, Ienaga *et al*. observed a zero-bias anomaly due to

the Fano resonance in Ni nanoconstrictions made by a MCBJ technique and showed the anomaly retains in large scale constrictions exhibiting the ferromagnetic properties [10].

In the present study, we measure the electrical conductance of Co constrictions with changing its size by a MCBJ technique to examine the size dependence of the Fano resonance in Co atomic-scale contact. A zero-bias anomaly is also found in Co atomic-scale contacts as well as in large constrictions like Ni nanoconstrictions [10].

2.   Experimental details

The sample wire, a ferromagnetic Co wire, which has a typical diameter of 0.25 mm with a purity of 99.99%, was intimately fixed on the top of the flexible phosphor-bronze substrate after making notch at the center by a commercial blade under a microscope and mounted in a triple point bending configuration in a vacuum chamber. After cooling at liquid helium temperature, the sample wire was stretched by bending the substrate mechanically.

Nanometer-scale contacts of Co were made by employing a homemade MCBJ technique [11]. A piezo element was then used to control the constriction size (a few 100 nm ~ atomic-sized) precisely. Thereafter, we have measured the spectra of differential conductance dI/dV as a function of the bias voltage using a lock-in technique with a frequency of 1 kHz. The whole experiment was performed at cryogenic environment, enabling to keep a stable contact for a long time by diminishing the thermal fluctuation. Besides, any contaminants at the contact are prevented in a cryogenic vacuum environment.

3.   Results and Analysis

By the repetition of making and breaking the contacts around two thousand times in a controlled way, the conductance histogram is built to study the atomic contacts as illustrated in Fig. 1(a). The position of the first peak at around $1.6G_0$ corresponds to the conductance of a single-atom contact, where $G_0 = 2e^2/h$ is the quantized unit of electrical conductance. The result is good agreement with previous theory and experiment done under similar conditions [9,12]. Further, the conductance histogram shows no fractional quantization which observed in atomic contacts of pure magnetic (Fe, Co and Ni) and nonmagnetic (Pt) metals by C Untiedt *et al*. [13].

To confirm the emergence of zero-bias anomaly in Co atomic-scale contacts reported by Calvo *et al*., we have measured the zero-bias conductance and dI/dV spectra for hundreds of atomic-scale contacts from $5G_0$ to the final stage of breaking such as those shown in Fig. 1(b) and (c), respectively. It is significant that most of the spectra show Fano-like features such as dip, tip or asymmetric shapes at around zero bias. Similar features are observed in

spectroscopy measurements for single magnetic adatoms on nonmagnetic surfaces [7], in molecular devices [14] and in Ni nanoconstrictions [10]. As the constriction is stretched, the zero-bias anomaly changes gradually in the same conductance plateau, while the shape of the dI/dV spectra changes remarkably at the jump of the conductance. Generally, the stretching induces a shift of the electron energy level in the contact due to a change of the overlap of the wave function, implying that the motion of the electrodes gives rise to a similar behavior as that observed in the gate-voltage effect in quantum dot and molecular device systems [3,14].
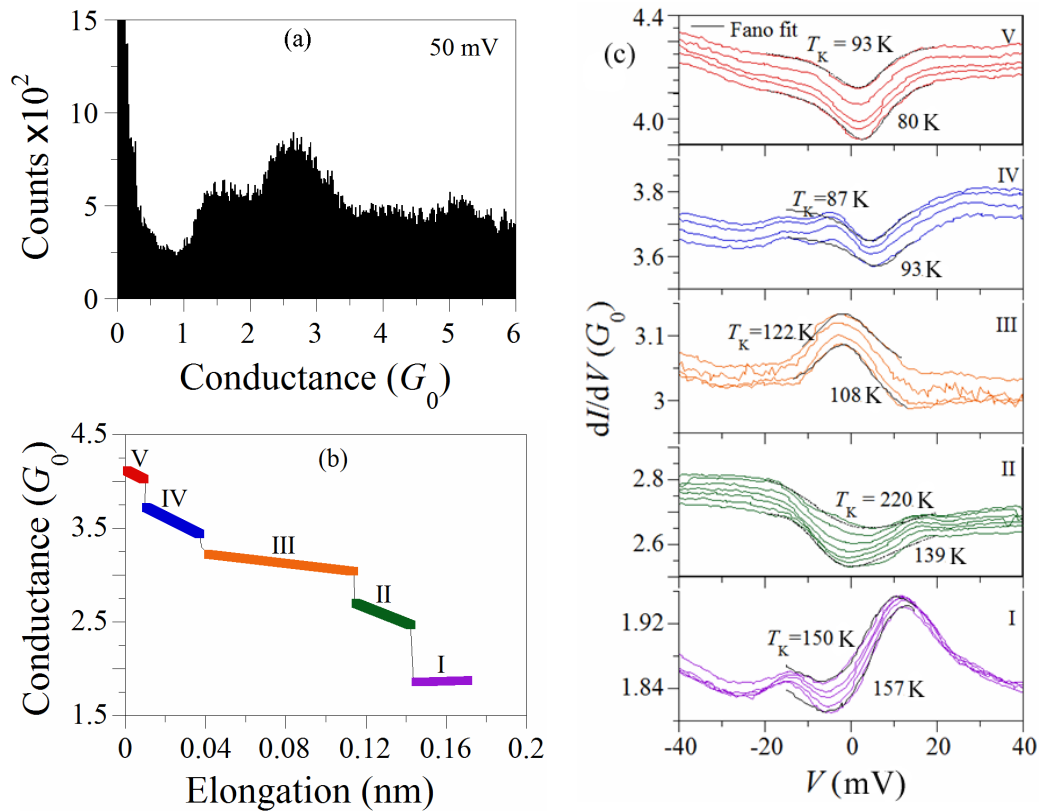

Fig. 1. (colour online) (a) The histogram depicted for around two thousands of conductance traces at 4.2 K; (b) Illustration of the zero-bias conductance for a monotonic elongation of Co nanocontact until the final stage of breaking; (c) Corresponding dI/dV spectra measured as a function of bias voltage according to the five regions observed in (b). The black lines obtained by fitting with the Fano formula (1).

It is well-known that a Fano resonance originates from the quantum interference between a discrete state and the continuum which can be represented as a mixing of two different configurations [8]. To analyze such resonance, it is important to fit the low bias conductance ($|eV| \leq \Gamma_K$) by the Fano formula:

$$G(V) = \frac{1}{G_0}\frac{dI}{dV} = g_{\text{off}} + \frac{A}{1+q^2}\frac{(q+\varepsilon)^2}{1+\varepsilon^2}$$

(1),

where $\varepsilon = \left(eV - \varepsilon_{K}\right)/k_{B}T_{K}$ is the bias shifted with respect to the center of the resonance ε_{K} and normalized by the natural width of the resonance $k_{B}T_{K}$; k_{B} is the Boltzmann's constant, T_{K} is the fitting parameter; q is the dimensionless Fano parameter that determines the shape of the Fano resonance and A is the amplitude of such resonance. By fitting these spectra at around $V = 0$ mV, we obtained the variation of T_{K} from 80 to 220 K that is almost similar agreement in the previous work performed by STM [7,9].

Additionally, the statistical analysis of the data is effective to obtain the origin of T_{K} for the resonances in atomic-scale contacts. We have constructed the histogram of T_{K} from fittings of more than two hundreds of atomic contacts, which is shown in Fig. 2. Obviously, the histogram follows a log-normal distribution, namely the natural logarithm of T_{K} is normally distributed. This indicates that the distribution is understood by assuming the Kondo model, where the Kondo temperature T_{K} varies exponentially with the coupling parameter J_{cd} between conduction electrons and d electrons and the density of states at Fermi energy $D(E_{F})$ as shown in the following formula:

$$T_{K} = \frac{W}{k_{B}} \exp\left[-\frac{1}{J_{cd}\, D\left(E_{F}\right)}\right] \tag{2},$$

where W is the bandwidth. These parameters J_{cd} and $D(E_{F})$ are determined by the local properties of the constrictions, which show normal distributions. The fitting of T_{K} histogram yields a most frequent value for the resonance width corresponding to $T_{K} = 90$ K, which is reasonable agreement with the previous results reported in [7,9]. As described above, it is important to consider that the origin of the Fano resonance in Co atomic-scale contacts is caused by the Kondo effect as pointed out by Calvo *et al*.
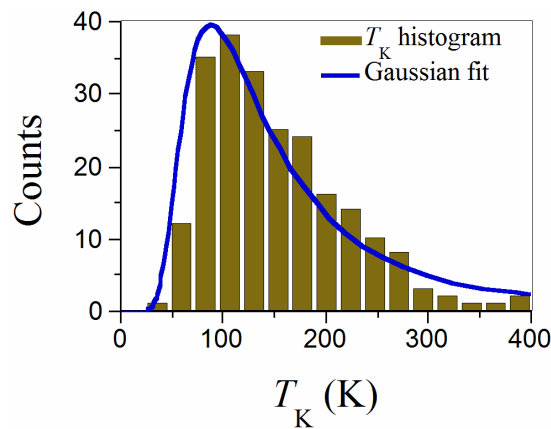

Fig. 2. (colour online) Histogram of T_{K} for more than two hundred fittings of Co atomic contacts. The solid (blue) line indicates the fit of the data to the log-normal distributions of T_{K} estimated below $6G_{0}$.

As mentioned above, the Fano resonance is survived in Ni nanoconstrictions where the bulk ferromagnetic properties are expected. To identify whether the similar feature appears in Co, we measure dI/dV spectra in large scale constrictions. Fig. 3 illustrates the size dependence of dI/dV spectra up to $85G_0$. Although the depth of the anomaly reduces by increasing the size of the constrictions, a dip shape anomaly is fitted by the Fano formula as shown by the solid black lines in Fig. 3. Due to the suppression of the depth of anomaly, we have enlarged the dI/dV spectra at $V \leq 20$ mV. Indeed, the Kondo temperature T_K gradually decreases and becomes constant because of reducing effect of both the parameters J_{cd} and $D(E_F)$ by increasing the contact size. The spectra imply that the ferromagnetic order and Kondo effect can coexist in Co nanoconstrictions as in the case of Ni ones.
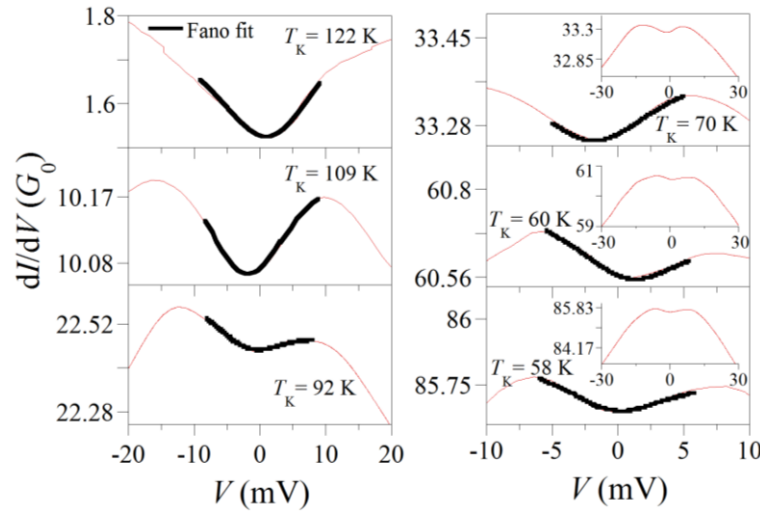

Fig. 3. (colour online) Spectra of dI/dV for large sized constrictions until $85G_0$. The insets in the right panel show the whole spectra. Solid lines indicate calculated Fano profiles with T_K.

Finally, we discuss the origin of the Kondo effect. Fig. 1 represents that a slight variation of the spatial geometry of the Co constrictions induces a change of the Kondo resonance spectra markedly. This suggests that the geometry is strongly associated with the appearance of the Kondo effect as in the case of Ni nanoconstrictions, in which a bridge-like structure where a Ni atom is placed on the Ni chain or surface like a bridge plays a crucial role for the existence of Kondo effect [10]. Generally, the magnetic moment of the bridge atoms should be varied from the bulk value due to the formation of an anisotropic structure in the crystal environment. Accordingly, a bridge-like atom forms a localized level, leading to the antiferromagnetic Kondo coupling J_{cd} due to the hybridization with the conduction electrons. The importance of the spatial geometry for the conductance is also pointed out by theoretical studies [15,16]. For instance, in Co adatom on the Cu(100) surface, the zero-bias anomaly due to Fano resonance appears in terms of the interference between the s and d_z^2 orbitals [16].

4. Conclusion

The spectra of dI/dV for Co monatomic contacts have been studied using MCBJ by the successive change of the geometry due to the stretching. Most of the spectra exhibit Fano-like features at around zero bias. The histogram of Kondo temperature follows a log-normal distribution that satisfies the normal distribution of their electronic properties in monatomic contacts. The size dependence of dI/dV spectra obtained in Co constrictions, suggest the existence of Kondo effect in ferromagnetic phase.

Acknowledgement

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