Transport and Magnetic Properties of Magnetic Alloy Atom Bridge

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Abstract

We have investigated the transport and magnetic properties of the atom bridge made from magnetic materials, which is the atom-scale wire constructed between a scanning tunneling microscopy tip and a solid surface, with ab initio calculations. In the case of FeNi alloy bridges, we have found that the atoms in the bridges can be designed to have significantly larger magnetic moment than that in the corresponding alloy bulk. We discuss about the origin of their transport properties in order to design the spin-polarized electron current through the bridges.

Key words: magnetic property ; quantum conductance ;nanowire ; scanning tunneling microscopy

In order to establish a basis for atom bridge related nano-spin-electronics, we have investigated the transport and magnetic properties of atom bridges made from magnetic materials experimentally [1] and theoretically by the use of the Hubbard model [2], and by performing the First-Principles calculations, within the density functional theory [3,4]. In our previous study [4], we have found that the magnetic state of the bridge can change by compressing the bridge in length. In the case of an Fe atom bridge with a twisted ladder structure, when the distance, d, between nearest neighbor atoms along the axis of the bridge, is longer than 1.10Å, the magnetic state of the bridge stays in a high-spin ferromagnetic state (the magnetic moment of the bridge, $M \sim 3\mu_{\rm B}$/atom). When $d < 1.10$Å, the magnetic state of the bridge is in a paramagnetic state. The single atom chain bridge is not as stable as those having the twisted ladder structure to show such a magnetic state change [3].

In Ref.[5], we have also investigated the magnetic properties of magnetic alloy bridges. In the case of an $Fe_{1-x}Ni_x$ atom bridge with a twisted ladder structure with $d = 1.75$Å, which is the (001) layer spacing of the Ni bulk, we have found that the atoms maintain a considerably large magnetic moment (about 3 $\mu_{\rm B}$ for an Fe atom and about 0.9 $\mu_{\rm B}$ for a Ni atom), and that the mean magnetic moment per atom in the bridge decreases linearly as x increases. These results indicate that due to the large distance between the Fe atoms and Ni atoms in our alloy atom bridge, the interactions between the atoms are not so effective to cause a considerable change in the electron states around the atoms. In this article, we present the results of our investigation on the transport properties of these magnetic alloy atom bridges.

The calculation results, presented in this article, are based on the density functional theory, using generalized gradient approximation (GGA) for the exchange-correlation energy, and given by a plane-wave and pseudopotential code, DACAPO. We assume that our atom bridge has a twisted ladder structure, as shown in the upper panel of Fig. 1, where each step in the upper side of the ladder crosses over its nearest-neighbor step in the lower side of the ladder. For simplicity, we assume that the bridge is infinitely long. We use the model structures of the ordered $Fe_{1-x}Ni_x$ alloy atom bridges of $x = 0.00$ shown in Fig.1 (a), $x = 0.25$ (b), $x = 0.50$ (c) and $x = 1.00$ (d) with $d = 1.75$Å. Positions of the atoms perpendicular to the bridge axis are optimized in terms of the total energy for each model structure.

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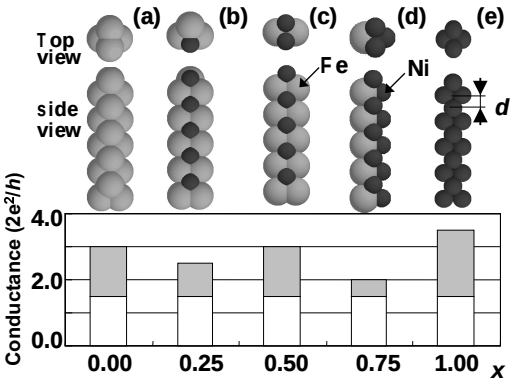

Fig. 1. Schematic description of the model structures for a pure Fe atom bridge (a), an $Fe_{7.5}Ni_{2.5}$ atom bridge (b), an $Fe_{0.5}Ni_{0.5}$ atom bridge (c), an $Fe_{0.25}Ni_{0.75}$ atom bridge (d) and a pure Ni atom bridge (e) (upper panel). The distance between nearest neighbor atoms in the z direction, d, is 1.75 Å. Conductance through the bridges (lower panel) which is contributed from the subbands for the majority spin electron (open rectangle) and minority spin electron (solid rectangle).

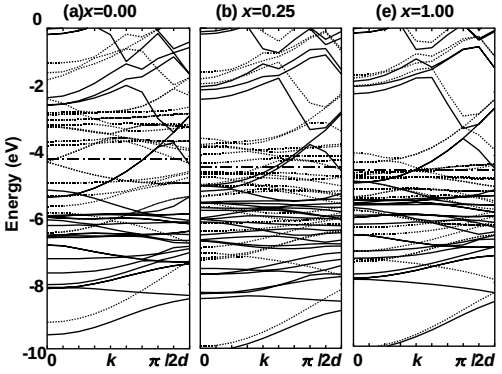

Fig. 2. Subband structures of a pure Fe atom bridge (a), an $Fe_{7.5}Ni_{2.5}$ atom bridge (b) and a pure Ni atom bridge (e). The subbands for the majority (minority) spin electron are plotted by the solid (broken) curves. The Fermi level is plotted by dashed line.

The details about the calculation are given in Ref.[5].

In the lower pannel of Fig. 1, we show the conductance estimated from the number of the subbands intersecting the Fermi level. In the figure, we can see that the conductance contributed from the minority spin electron changes and that from majority spin electron does not change as x changes.

In Fig. 2, we show the subband structures of the pure Fe (a), $Fe_{0.75}Ni_{0.25}$ alloy (b) and pure Ni (e) atom bridges. The subband structure of the majority spin electron is rather rigid, and only the s-like bands of them intersect the Fermi level. The degeneracy of these subbands are slightly lifted by the broken symmetry in the case of the alloy bridge (b). But this energy separation is so small and the number of the majority spin electron subband intersecting the Fermi level does not change. Then the conductance contributed from the majority spin electron subbands does not change as x changes from 0 to 1. On the other hands, the subband structure of the minority spin electron near the Fermi level is strongly affected by the Fe-Ni atom mixing. Whether the electron current is spin-polarized or not depends only the subband structure of the minority spin electron near the Fermi level, in which there is the potentiality to design the spin-dependent quantized conductance and/or spin-polarized current. For example, the electron current through the bridges (a) and (c) is not spin-polarized, and that through the bridges (b) and (d) is spin-polarized toward the direction of the magnetization of the atom bridge. Moreover the current through the bridge (e) is spin-polarized toward the opposite direction of the magnetization of the atom bridge, which has been shown in the case of a single Fe linear chain bridge [4].

We think that such information is important and useful in order to establish a basis for realizing atom bridge related nano-spin-electronics.

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