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Electronic and transport properties of noncollinear magnetic monatomic Mn chains: Fano resonances in the superlattice of noncollinear magnetic barriers and magnetic anisotropic bands

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ABSTRACT

By means of the density functional theory combined with non-equilibrium Green's function method, ballistic transport properties of one-dimensional noncollinear magnetic monatomic chains were investigated using the single-atomic Mn chains as a model system. Fano resonances are found to exist in the monatomic Mn chains with spin-spiral structure. Furthermore, in the monatomic Mn chains with magnetic soliton lattice, Fano resonances are enhanced and cause the conductance splitting in the transmission spectra. The Fano resonances in the noncollinear magnetic single-atomic Mn chains are arising from the coupling of the localized *d*-states and the extended states of the quantum channels. By constructing a theoretical model and calculating its conductance, it is found that the phenomena of Fano resonances and the accompanying conductance splitting exist universally in the superlattice of one-dimensional noncollinear magnetic barriers, due to the interference of the incident waves and reflected waves by the interfaces between the neighboring barriers. Moreover, the band structures of the ferromagnetic and spin-spiral monatomic Mn chains exhibit a strong dependence on the spatial arrangement of the magnetic moments of Mn atoms when spin–orbit coupling is considered.

1. Introduction

One-dimensional (1D) transition metal (TM) monatomic chains and nanowires have received much attention for both the meaning of fundamental physics [1–6] and the potential applications in atomic-scale magnetic devices and spintronics in the future [7–9]. According to the recent theoretical and experimental results, many 1D TM monatomic chains exhibit a noncollinear magnetism, especially the spin-spiral ground state [8, 10–12]. For example, Co singe-atomic chains on monatomic layer of Mn on W(110) were investigated by spin-polarized scanning tunneling microscope and found to have a spin-spiral structure (SS) [8]. From the work of Tung et al. and Schubert et al., stable SSs are also predicted to exist in both the free standing V, Mn, and Fe monatomic chains [10] and the single-atomic alloying chains of Mn, Fe, and Cr [11]. On the other hand, under the magnetic field perpendicular to the helical axis, the periodic SS will turn into another noncollinear magnetic order which is called magnetic soliton lattice (MSL) [13–15]. This transition from SS to MSL has been studied experimentally in magnetic crystals of $Cr_{1/3}NbS_2$ [16].

Recently, an experimental result revealed that the magnetoresistance (MR) along the axis in the chiral magnetic crystal of $Cr_{1/3}NbS_2$ can be attributed to the magnetic scattering of conduction electrons by the MSL [17]. This result suggests that noncollinear magnetism, such as SS and MSL, may result in some nontrival transport properties for the 1D or quasi-1D atomic-scale structures. From this point of view, it is necessary to study the scattering effect of the noncollinear magnetism on the electronic transport properties of 1D TM single-atomic chains for the promise of the spintronics devices and atomic-scale devices in the future application.

As a typical 1D TM single-atomic chain, monatomic Mn chains (MMCs) have been studied both experimentally and theoretically in recent years [9–12]. MMCs of up to ten atoms were created on an insulating CuN/Cu(001) surface using scanning tunneling microscope experimentally [9]. On the other hand, both freestanding MMCs and supported MMCs on Cu(110) and Ag(110) are predicted to have a spin-spiral ground state from previous computational results [10–12]. Based on above results, MMCs, as a model system of 1D monatomic chains, constitute a unique research category for

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fundamental physics and applications in the atomic-scale devices.

In this paper, ballistic transport properties of SS and MSL in MMCs were investigated by means of first-principle calculations combined with the non-equilibrium Green's function (NEGF) method. Owing to the existence of SS, the Fano resonances [18,19] are found in the transmission spectra of MMCs with SS. Moreover, the Fano resonances are enhanced in the MMCs with MSL and bring the conductance splitting in their transmission spectra. By constructing a theoretical model and calculating its conductance, Fano resonances and accompanying conductance splitting are found to exist universally in the superlattice of one-dimensional noncollinear magnetic barriers, therefore are expected to occur in other 1D or quasi-1D nanoscale systems with SS and MSL. Finally, we consider the effect of spin–orbit coupling (SOC) on the band structure (BS) and transmission spectrum of MMCs with SS, for that SOC usually leads to unique phenomena, such as magnetic anisotropic BS and MR [20–26].

This paper is organized as follows. In Section 2, we introduce the geometry structures (Section 2.1) and the details of first-principle calculations (Section 2.2). In Section 3, we discuss the transport properties of the noncollinear magnetic MMCs. In Section 4, a theoretical model of noncollinear magnetic MMCs is constructed to study the electron transport in the superlattice of noncollinear magnetic barriers. The BS and transmission spectra of spin-spiral MMCs are discussed in Section 5, with considering the effect of SOC. We summarize our work and give the conclusions in Section 6.

2. Junction structures and computational details

2.1. Junction structures

In this work, we consider the transverse spin-spiral MMCs, where all the spins rotate in a plane perpendicular to the chain axis. Therefore the number of total Mn atoms in each period (n) and the angle between the magnetic moments of adjacent atoms (θ) have a simple numerical relation of $n=360\,m/\theta$ (m is the smallest integer to keep n is an integer) and θ can be used to distinguish the chains. The distance of nearest Mn atoms is fixed to be 2.4 Å, which is the bond length of the ground state of free-standing MMCs [10,12]. In order to calculate the transmission spectra of SS in MMCs, we construct spin-spiral junctions (SSJs) by attaching the spin-spiral MMCs to two semi-infinite ferromagnetic (FM) MMCs. Fig. 1(a) presents a SSJ with $\theta=90°$ (90°-SSJ), which contains a SS with $\theta=90°$ (90°-SS) in the effective scattering region. As shown in Fig. 1(a), the magnetic moments of two FM electrodes are parallel to each other. In order to improve the matching of the SS and the electrodes, two matching regions (L0 and R0 in Fig. 1) are included in the effective scattering region and used to connect the SS and two leads. Each matching region contains four Mn atoms and the magnetization of the matching regions is parallel to that of the electrodes. For all the junction structures in this work, the electrodes and the matching regions are the same as that are shown in Fig. 1(a). We change θ from 0° to 162°, in steps of 18°, to investigate the scattering effect of SS in MMCs. In particular, when θ equals to 0°, all magnetic moments of the Mn atoms have the same directions, therefore the 0°-SSJ is a FM monatomic junction structure (FMJ). For comparison, we also

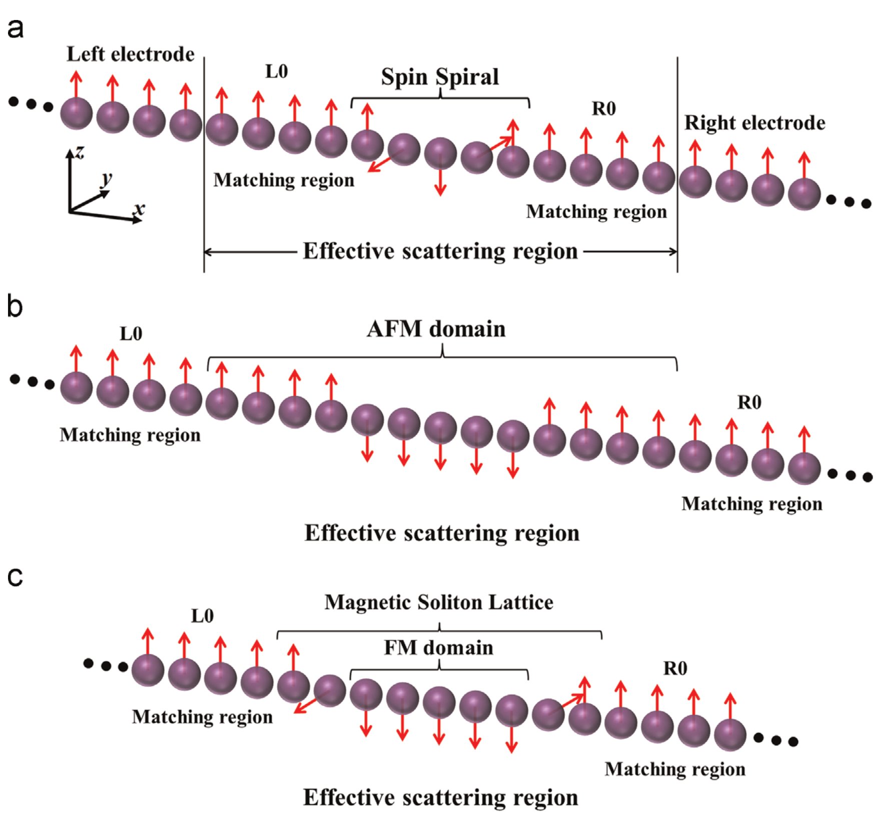

Fig. 1. Noncollinear magnetic junction structures. (a) The 90°-SSJ, a SS with $\theta=90°$ is in the effective scattering region. Considering that the matching regions and the electrodes of all the junctions in this work are the same as that are shown in (a), only the effective scattering regions of AFMJ and MSLJ are shown here. (b) The AFMJ, where the magnetic moments of central five Mn atoms are antiparallel to that of other Mn atoms. (c) The MSLJ, which contains a forced FM domain constituted by five Mn atoms.