Recent experiments in ferromagnetic atomic-sized contacts have shown that the anisotropic magnetoresistance (AMR) is greatly enhanced and has an asymmetric angular dependence as compared with that of bulk samples. The origin of these effects is still under debate. In this work we present a theoretical analysis of the AMR in atomic contacts of the 3d ferromagnetic materials. Our results strongly suggest that the anomalous AMR stems from the reduced symmetry of the atomic contact geometries. We also present calculations supporting the idea that the pronounced voltage- and temperature dependence in some experiments can be attributed to impurities near the constrictions.

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with saturated magnetization. We use the SOC constant $\xi_i = 70$ meV, which is the experimental value for Ni. We stress that, while this type of model is not expected to be as accurate as \textit{ab initio} counterparts, it captures the essential physics. It also has the advantage that it allows us to analyze phenomena like BAMR in realistic contact geometries, which is currently outside the scope of \textit{ab initio} methods.

In order to describe the electronic transport we use the nonequilibrium Green’s function formalism \cite{15}. Briefly, the atomic contacts are divided into three parts, a central region $C$ containing the constriction and the left/right ($L/R$) leads, which we model as infinite surfaces. The retarded Green’s functions of the central part read

$$G_{CC} = \left[ \varepsilon S_{CC} - H^{(0)}_{CC} - H^{(SO)}_{CC} - \Sigma_L - \Sigma_R \right]^{-1}, \quad (2)$$

where $\Sigma_X = t_{CX} g_{XX} t_{CX}^\dagger$ are the lead self-energies ($X = L, R$). Here, $t_{CX} = \varepsilon S_{CX} - H^{(0)}_{CX}$, with $H^{(0)}_{CX}$, $S_{CX}$ the hopping elements and overlaps between the $C$ region and the lead $X$, and $g_{XX}$ is a surface Green’s function. In general $H^{(0)}$ and $\Sigma_{L,R}$ depend on the bias voltage $V$. The $V$-dependent transmission matrix is $t(\varepsilon, V) = \Gamma_{L}^{1/2} G_{CC} \Gamma_{R}^{1/2}$, where $\Gamma_X = i(\Sigma_X - \Sigma_X^\dagger)$. The current then adopts the standard Landauer-Büttiker-like form

$$I(V) = \frac{e}{h} \int_{-\infty}^{\infty} d\varepsilon \tau(\varepsilon, V) \left[ f_{L}(\varepsilon, V) - f_{R}(\varepsilon, V) \right], \quad (3)$$

where $f_{L,R}$ are the Fermi functions and $\tau(\varepsilon, V) = \text{Tr} \left[ t^\dagger t \right]$ is the transmission function. The low-temperature linear conductance can be written as $G = (e^2/h) \sum_n \tau_n$, where $\tau_n$ are the transmission coefficients, i.e. the eigenvalues of $t^\dagger t$ at Fermi energy $\varepsilon_F$.

In the calculations presented here we have neglected the SOC in the leads. We have checked that this only introduces a small change in the contact resistance that does not alter the conclusions but reduces the computation time enormously. On the other hand, we determine self-consistently the on-site energies of the atoms in the constriction by imposing the local charge neutrality that metallic elements should exhibit.

We now apply this method to calculate the conductance of Ni atomic contacts. First we consider an ideal geometry with the atoms kept fixed on fcc lattice positions and forming pyramid-like tips in the [111] direction that end in a common central atom [Fig. 1(a)]. In Figs. 1(b,c) the conductance and its channel decomposition as function of $\theta$ for several values of $\phi$ are shown. Surprisingly, the conductance of this one-atom contact exhibits the bulk-like AMR with a $\cos^2 \theta$ dependence (minimum at $\theta = 0$), an amplitude of $0.5\%$ and practically no dependence on $\phi$. In fact, the individual channels show a more complicated dependence on $\theta$, and the amplitude of variation for one channel can be bigger than that of the total conductance, but in the latter these features cancel and the $\cos^2 \theta$ dependence is recovered.

It seems obvious that the cancellation is related to the high symmetry of the ideal geometry. To test this idea we have distorted the contact by shifting randomly the atomic positions by up to $5\%$ of the nearest-neighbor distance [Fig. 1(d)]. As seen in Fig. 1(e), the individual channels now show roughly the same amplitude of variation with $\theta$ as in the ideal contact, but due to the disorder they exhibit a more complex $\theta$ dependence, and a strong dependence on $\phi$. As a consequence, the contributions of the channels no longer cancel out and the AMR can have a different amplitude, with the conductance extrema shifted in $\theta$ and with a strong dependence on $\phi$ [Fig. 1(f)]. This example illustrates that the origin of the anomalous angular dependence and amplitude of the AMR in atomic contacts can be simply the reduced symmetry of these junctions together with the fact that the conductance is mainly determined by a few atoms in the narrowest part of the constrictions. We want to point out that we have found similar results for Co and Fe atomic contacts, which confirms this conclusion \cite{15}.

![Figure 1](image-url)

FIG. 1: (Color online) (a) Ideal Ni one-atom contact in fcc [111] direction with atoms on lattice positions. Green atoms are those in the atomic constriction, yellow ones are part of the surfaces used to model the leads. (b,c) Channel decomposition and the total linear conductance as a function of $\theta$ for different angles $\phi$. The relative conductance is defined as $G_{rel} = G(\theta, \phi)/G(\theta, \phi)_\theta = 1$. (c) Channel decomposition of (b). (d)-(f) Same as (a)-(c), but with the contact distorted by randomly shifting the red atoms by up to $5\%$ of the nearest-neighbor distance.
Since the geometry plays such a prominent role in the AMR, it is important to determine the geometries that can be realized in an actual experiment. For this purpose, we have carried out classical MD simulations of the formation of Ni atomic contacts, following Ref. [14]. An example of the contact evolution is shown in Fig. 2. Here, we start with an ideal Ni bar containing 112 atoms on lattice sites in fcc [001] direction. The bar is attached to rigid surfaces that are separated in a stepwise manner, simulating the elongation process of a break junction. In Fig. 2(a) we show the evolution of the spin-projected and total conductance during elongation in the absence of SOC. Adding SOC introduces only a small change in the averaged total conductance. As usual, the sudden atomic rearrangements are reflected as steps in the conductance [1]. The vertical lines refer to the geometries of Fig. 2(b) obtained during the elongation. For them we have computed the dependence of the conductance on θ and φ, and the results are shown in Fig. 2(c). For contact 1, which is just an elastic deformation of the ideal contact, the conductance has two types of behavior depending on φ: one is cos²θ-like, while the other is clearly more complex. In order to visualize the overall angular dependence, we show the relative AMR on a “Bloch sphere” [Fig. 2(d)]. The contact 1 and hence its AMR have an approximate four-fold symmetry. When deformations emerge in the contact, the angular dependence becomes irregular and strongly dependent on φ. For example, for contact 2 there is a strong variation of AMR with φ, and depending on its value, the AMR amplitude can be almost one order of magnitude larger than in the bulk limit or cancel almost entirely. As the contact evolution proceeds, the AMR has an amplitude of around 2%. In almost all cases, the conductance is not only shifted in θ, but it also has a more complicated behavior than just cos²θ. Approaching the tunnel regime (G < 0.1e²/ℏ), we do not observe a further increase of the AMR amplitude, contrary to experiments [3]. One reason may be that the isolated tip atoms in tunneling regime exhibit a finite orbital moment [16] (not considered here), which may lead to a local deviation of the spin-quantization axis from the field direction and an additional increase in resistance. Finally, in the limit of thick contacts, we recover bulk behavior with an amplitude of 0.45%, as shown in Fig. 2(e). The statistical analysis of all contact geometries shows an increase of AMR to 2% on average in the last steps before breaking, see inset of Fig 2(a). This confirms that the lack of symmetry in atomic contacts gives rise to the enhancement of the AMR signal.

We have not found indications of tip resonances, which are present in ideal one-dimensional geometries [17, 18] and which were suggested as the origin of the experimental findings [17]. For example, the transmission for the contact of Fig. 2(a) has almost no structure around ε_F on the scale of millielectronvolts, as shown in Fig. 3(a). We thus believe that the voltage and temperature dependences reported in Refs. [3, 10] are indeed associated with impurities close to the constriction, as reported earlier for non-magnetic junctions [19, 20]. Following Ref. [20], one may estimate that the reported [3] voltage period of a few millivolts can stem from impurities located hundreds of nanometers away from the contact. Such length scales cannot be modeled realistically, but we have developed a toy model to support the idea. As represented schemat-
The relative variations shown in Fig. 3(e) bear a striking resemblance to the experimental results of Ref. [3]. Finally, we show in Figs. 3(f,g) the temperature dependence of both the linear and non-linear conductance. The effect of temperature is to smooth the 0 K characteristics, again compatible with the experimental observations [10].

In summary we have shown that the anomalous magnitude and angular dependence of the AMR in ferromagnetic atomic-sized contacts can be explained naturally in terms of the reduced symmetry of the atomic junction geometries. We predict a strong anisotropy of the conductance channels, but have not found any signature of BAMR. We have presented a simple model which illustrates that the pronounced voltage and temperature dependence found in some experiments may originate from the presence of impurities close to the constriction.

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