Exchange interactions and Néel temperature of a Fe monolayer on W(001): A first-principles study

L. M. Sandratskii, E. Şaşıoğlu, and P. Bruno
Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle, Germany
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The density-functional study of the magnetic properties of a single Fe monolayer on W(001) is reported. The system possesses, presently unique for Fe layers, antiferromagnetic structure. We demonstrate that the study of the instability of the ferromagnetic state predicts the ground-state antiferromagnetic structure. We use the frozen-magnon technique to evaluate the interatomic exchange parameters for different reference states. The relative role of the Fe-Fe and Fe-W exchange interactions is revealed. The Néel temperature is estimated.

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I. INTRODUCTION

The magnetic state of artificially fabricated materials is one of the main factors determining the range of possible applications of these systems. Also from the viewpoint of understanding of fundamental principles of condensed-matter magnetism, the study of artificial materials is an important and challenging field. Recently Kubetzka *et al.*,[1] reported an unusual magnetic behavior of the Fe monolayer (ML) on W(001). The spin-polarized scanning tunneling microscopy measurements detected the antiferromagnetism of the Fe film where the magnetic compensation takes place within the layers. The first-principles calculation of the total energy of the antiferromagnetic (AFM) and an assumed ferromagnetic (FM) structures confirmed that the antiferromagnetic configuration has lower energy.[1,2] This result is in correlation with earlier calculation by Wu and Freeman[3] who also reported the antiferromagnetic state of the Fe ML on W(001). Since an unsupported Fe monolayer with the same lattice spacing has a ferromagnetic ground state,[2] the role of the Fe-W hybridization becomes evident.

The purpose of the present paper is to gain further insight into the unique magnetism of the Fe layer on W. The fact that the total energy of the ferromagnetic state is higher than the energy of the AFM state does not exclude that the FM configuration corresponds to a local minimum of the energy as a function of the directions of atomic moments. Such a "metamagnetic"[4] energy landscape can be useful for applications making possible the stabilization of various magnetic states. Using the frozen-magnon approach we study the stability of magnetic configurations and estimate the interatomic exchange parameters. We compare the relative strength of the Fe-Fe and Fe-W exchange interactions. The calculated exchange parameters are employed to estimate the Néel temperature.

II. CALCULATIONAL TECHNIQUE

Within the density-functional theory (DFT) the interatomic exchange parameters are given by the second derivatives of the energy with respect to the deviations of the magnetic moments (see, e.g., Ref. 5). These derivatives are taken at a magnetic configuration where the first derivatives are zero. The condition on the first derivatives is always fulfilled by the ground-state magnetic configuration providing the global minimum of the total energy. Also the magnetic configurations corresponding to local minima, global or local maxima, or saddle points can be used as the reference state for the estimation of exchange parameters. In the case the spin-orbit coupling is neglected, the first derivatives vanish for any collinear magnetic configuration. This is a consequence of the symmetry of the problem. Therefore any collinear configuration can be used as a reference state.

The DFT calculations reported in the paper are performed in the scalar-relativistic approximation within the ASW method with the use of the atomic-sphere approximation.[6] The generalized gradient approximation to the energy functional is employed.[7] The Fe ML on W(001) was modeled by the supercell containing nine layers of W, one Fe layer and four layers of empty spheres. The experimental W lattice constant $a=3.165$ Å was used. For the distance between the interface W and Fe layers we used the theoretical relaxed value of 2.44 a.u. reported in Ref. 1.

To evaluate the interatomic exchange interactions we map the system onto a classical Heisenberg Hamiltonian

$$H_{\text{eff}} = -\sum_{i \neq j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j \qquad (1)$$

where J_{ij} is an exchange interaction between two atomic moments and $\mathbf{s}_i$ is the unit vector pointing in the direction of the magnetic moment at site i. The mapping is performed by the calculation of the energies of the so-called frozen-magnon magnetic configurations[8] and the selection of the Heisenberg parameters that reproduce these energies.

We begin with the consideration of the ferromagnetic Fe ML. The frozen-magnon states are determined by the expression

$$\mathbf{e}_n = [\cos(\mathbf{q} \cdot \mathbf{R}_n)\sin\theta, \sin(\mathbf{q} \cdot \mathbf{R}_n)\sin\theta, \cos\theta], \qquad (2)$$

where $\mathbf{R}_n$ are vectors of the two-dimensional lattice, $\mathbf{q}$ are magnon wave-vectors belonging to the two-dimensional Brillouin zone, $\mathbf{e}_n$ is the unit vector in the direction of the magnetic moment at site $\mathbf{R}_n$, polar angle θ gives the deviation of the moments from the axis of net magnetization. Within the Heisenberg model (1), the energy of frozen-

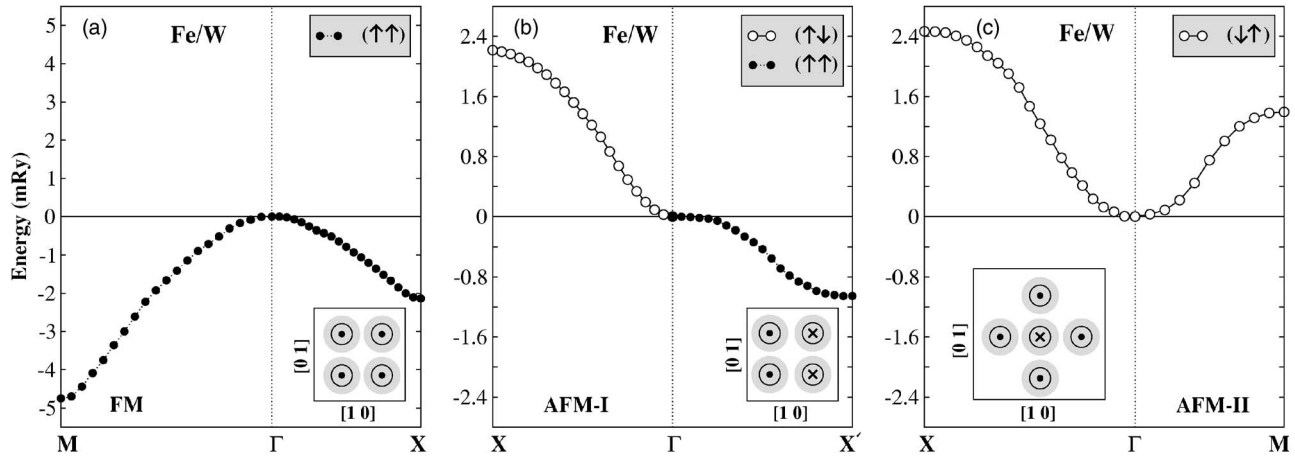

FIG. 1. The frozen-magnon energies for Fe ML on W(001) along two lines in the 2D Brillouin zone for three different magnetic reference states: (a) ferromagnetic, (b) antiferromagnetic with $\mathbf{q}=(1\,0)$ (AFM-I), and (c) antiferromagnetic with $\mathbf{q}=(1\,1)$ (AFM-II). Here and in the text all reciprocal-space vectors are given in units of π/a. The square inserts in the bottom part of the figures present the reference magnetic structure. Definitions of the points of the Brillouin zone in panels (a) and (b): $\Gamma(0,0)$, $M(1,1)$, $X(1,0)$, $X'(0,1)$. In panel (c): $M(\frac{1}{2},\frac{1}{2})$, $X(1,0)$. In cases (a) and (c) the points (1,0) and (0,1) are equivalent. In case (b) they are not equivalent. The filled (open) circles show the frozen-magnon energies for the wave vectors parallel to the ferromagnetic (antiferromagnetic) rows of atoms.

magnon configurations can be represented in the form

$$E(\theta,\mathbf{q}) = E_0(\theta) + \sin^2\theta J(\mathbf{q}), \tag{3}$$

where E_0 does not depend on $\mathbf{q}$ and $J(\mathbf{q})$ is the the Fourier transform of the interatomic exchange parameters

$$J(\mathbf{q}) = \sum_{\mathbf{R}} J_{0\mathbf{R}} \exp(i\mathbf{q}\cdot\mathbf{R}). \tag{4}$$

The numerical experiments[8] have shown that in systems with well-defined atomic moments, Eq. (3) very well reproduces the first-principles total energies up to θ angles exceeding 30°. In the calculations we used $\theta=30°$. The total energies were evaluated on the basis of the magnetic force theorem.[9,10] In the calculations of the frozen-magnon energies 30×30 points in the two-dimensional Brillouin zone have been used.

A uniform meshes of the frozen-magnon wave vectors over the first Brillouin zone has been employed. The minimal number of the wave vectors was 144. Making the back Fourier transformation of the frozen-magnon energies we obtain the interatomic Heisenberg exchange parameters.

III. RESULTS AND DISCUSSION

A. Frozen magnon dispersions and exchange parameters

In Fig. 1(a), we show the frozen magnon dispersion calculated for the ferromagnetic reference state. For $\mathbf{q}\neq0$ all calculated frozen-magnon energies are negative manifesting the instability of the reference state. The lowest magnon energy is obtained for $\mathbf{q}=(1\,1)$ revealing the highest instability with respect to the formation of a magnetic structure with given $\mathbf{q}$. This result is in agreement with the experimental finding of the AFM structure with wave vector $\mathbf{q}=(1\,1)$ to be the ground state.

The interatomic Heisenberg exchange parameters corresponding to the ferromagnetic reference state are given in Fig. 2. The leading exchange interaction is the antiferromagnetic interaction between the nearest Fe atoms. The interactions between further neighbors are much weaker.

For comparison, the exchange parameters calculated for the ferromagnetic configuration of the unsupported Fe ML is also presented in Fig. 2. The two sets of exchange parameters differ drastically. The leading antiferromagnetic interaction between neighboring atoms of Fe ML on W(001) is replaced by a strong ferromagnetic interaction in unsupported ML. This makes the ground state of the unsupported ML ferromagnetic. The difference between the unsupported Fe ML and the Fe ML on W(001) reveals the crucial role of the

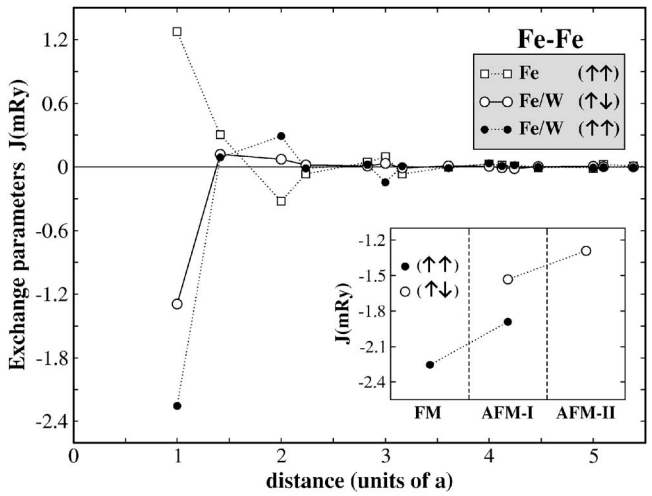

FIG. 2. The Fe-Fe exchange parameters of a free standing ferromagnetic Fe ML (open square), and for the FM (filled circles) and AFM-II (open circles) reference states of a Fe ML on W(001). The inset compares the nearest-neighbor Fe-Fe exchange parameters of Fe ML on W(001) for three different reference states. The exchange parameters correspond to the Heisenberg Hamiltonian of the form $H_{\text{eff}}=-\Sigma_{i\neq j}J_{ij}\mathbf{s}_i\cdot\mathbf{s}_j$.

TABLE I. Magnetic moments (in μ_B) for Fe ML on W(001) and the total energy difference $\Delta E = E - E_{[\text{AFM-II}]}$ (in mRy/atom) for Fe ML on W(001) and unsupported Fe ML.

	FM	AFM-I	AFM-II
		Fe ML on W(001)	
m_{Fe}	2.18	2.44	2.47
ΔE	9.36	1.99	0.00
		unsupported Fe ML	
m_{Fe}	3.41		3.46
ΔE	−17.96		0.00

Fe-W hybridization in the formation of the ground state of the ML.[2] Ferriani *et al.*, put forward the hypothesis that the strong Fe-W hybridization makes the interlayer Fe-W exchange interaction stronger than the intralayer Fe-Fe exchange interactions. To verify this hypothesis we estimated the strength of the Fe-W exchange coupling by calculating the parameter $J_{\text{Fe-W}} = \Sigma_{i_W} J_{0,i_W}$ where 0 corresponds to an iron atom and the sum runs over all W atoms. The induced moment in the first W layer is opposite to the Fe moments and assumes the value $0.29\mu_B$/atom. The induced moments in further W layers are much smaller.

Parameter $J_{\text{Fe-W}}$ characterizes the effective field experienced by an iron atom from the side of all W atoms. This parameter can be estimated by comparison of the total energies of two magnetic configurations: collinear one and the configuration where the Fe and W moments form a nonzero angle. The calculation gives $J_{\text{Fe-W}} = 1.1$ mRy. For comparison, the corresponding parameter describing the effective field on an iron atom produced by all other Fe atoms is 7.9 mRy. Therefore, the role of the Fe-W exchange interaction in the energetics of the magnetic configurations of the Fe ML is substantially smaller than the role of the Fe-Fe interactions. This result shows that the transition from the ferromagnetism of an unsupported Fe ML to the antiferromagnetism of the Fe ML on W(001) is governed by the strong variation of the Fe-Fe exchange interactions. This variation is caused by the W-Fe hybridization leading to strong change of the electronic structure of the Fe ML. Since the exchange parameters reflecting the energy price of the deviation of magnetic moments depend crucially on the electronic structure, the Fe-Fe exchange parameters also change strongly. (Below we discuss the relation between the electronic structure and exchange parameters in more details.) This scenario being in agreement with the conclusion of Ferriani *et al.*, concerning the crucial role of the Fe-W hybridization in the formation of the AFM ground state on the Fe ML on W(001) differs in the estimation of the relative roles of the Fe-Fe and Fe-W exchange interactions.

Having now established the instability of the ferromagnetic state we continue with the study of the antiferromagnetic configurations. The calculations are performed for two antiferromagnetic states characterized by vectors $\mathbf{q} = (1\ 0)$ and $\mathbf{q} = (1\ 1)$. The total energies and the values of the Fe moments are collected in Table I.

As expected from the dispersion of the ferromagnetic magnons (Fig. 1) and the corresponding exchange parameters (Fig. 2) the AFM-II structure has lower energy than the AFM-I structure. And the energies of the both AFM states are lower than the energy of the ferromagnetic configuration. The application of the Heisenberg exchange parameters obtained for the FM reference state to the estimation of the energy difference between FM and AFM-II states gives the value of 19.540 mRy/atom that is about twice the value obtained in the DFT calculation (Table I).

These results show that although the ferromagnetic frozen magnons determine properly the strongest instability with respect to the formation of the experimental ground-state structure AFM-II the corresponding interatomic exchange parameters do not describe quantitatively the energy difference of the FM and AFM-II configurations.

To study the stability of the antiferromagnetic configurations we calculate the frozen-magnon energies for the AFM-I and AFM-II states [Figs. 1(b) and 1(c)]. As expected for the ground state, the AFM-II configuration is stable with respect to the deviation of the atomic moments: all frozen-magnon energies are positive. The AFM-I configuration assumes an intermediate position between FM and AFM-II. The energies are positive for $\mathbf{q}$ parallel to the antiferromagnetic rows of atoms and negative for $\mathbf{q}$ parallel to the ferromagnetic rows. Thus the calculations of the frozen-magnon dispersions for different reference magnetic states provide a consistent picture of the instability of the parallel orientation of the nearest Fe moments and the stability of the antiparallel orientation.

In Fig. 2 we present the Fe-Fe exchange parameters[11] obtained by the back Fourier transformation of the frozen-magnon dispersions for the AFM-II reference state. The pattern of the interatomic exchange interactions is qualitatively similar to the pattern obtained for the ferromagnetic reference state: The strongest exchange interaction takes place between the nearest neighbors and has antiferromagnetic character. The interactions between further neighbors are much weaker. The quantitative comparison shows, however, a strong difference in the values of the exchange parameters. The leading exchange parameter calculated for the ground state is about 40% smaller than the corresponding parameter estimated for the FM state. For AFM-I, the interactions between atoms separated by vectors $(a\ 0)$ and $(0\ a)$ become different. The values of these parameters assume intermediate positions between FM- and AFM-II cases. The parameter $J_{(0a)}$ corresponding to the ferromagnetic rows have larger absolute value and is closer to the parameter obtained for the FM reference state (see inset in Fig. 2). Respectively, the parameter corresponding to the antiferromagnetic rows is closer to the value obtained for the ground antiferromagnetic state.

The difference of the parameters calculated for different reference states reveals the limits of the description of Fe ML on W(001) within the Heisenberg model. To estimate the value of the Néel temperature that will be our next purpose we need to select one set of the exchange parameters. By construction, the set obtained for the ground-state AFM-II structure provides the best description of the low-energy excitations. Applying this set of parameters to the evaluation of the energy difference for two strongly different magnetic configurations AFM-II and FM, we get the value of 9.76 mRy/atom that is close to the value of 9.36 mRy/atom

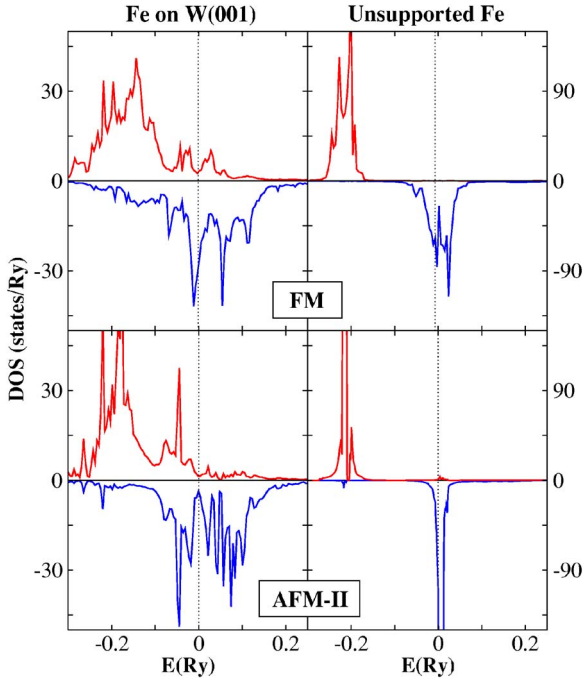

FIG. 3. (Color online) The spin-resolved Fe 3*d* DOS for Fe ML on W and unsupported Fe ML. The DOS are presented for FM and AFM-II configurations. The dotted lines mark the position of the Fermi level. The energy origin is selected at the Fermi level of the AFM-II structures. Therefore the Fermi energy of the FM structures somewhat deviates from zero. This deviation is −1.4 mRy for Fe/W(001) and is not noticeable in the figure. For unsupported Fe ML the deviation assumes a larger value of −7.2 mRy.

obtained in the DFT calculation. Thus the set of the exchange parameters corresponding to the AFM-II reference state suits well our purpose of the estimation of the magnetic transition temperature.

B. Densities of states

To get deeper understanding of the relation between electronic structure and exchange parameters we present in Fig. 3 the spin-resolved Fe 3*d* density of states (DOS) for the FM and AFM-II configurations of the Fe ML on W(001) and unsupported Fe ML. The comparison of the DOS shows that in the case of Fe ML on W the Fe 3*d* bands are much broader that reveals the importance of the Fe-W hybridization. For the unsupported ML, the AFM-II state has higher energy (Table I) reflecting ferromagnetic character of the leading interatomic exchange interactions in this case (Fig. 2).

Two trends can be distinguished in the variation of the electronic structure under transition from FM to AFM. In a ferromagnet, all atomic moments have the same direction. Therefore, the atomic spin-quantization axes are parallel to each other and to the global spin-quantization axis. As a result, the atomic spin-up and spin-down states do not mix. In the AFM case, the local atomic spin-up states of one sublattice and local atomic spin-down states of other sublattice have the same projection on the global spin-quantization axis and can hybridize with each other. This spin-mixing is the first trend connected with the transition from FM to AFM. The strength of the hybridization depends on the relative energy position of the states. If the exchange splitting exceeds the characteristic width of the bands the local spin-up and spin-down states lie in different energy intervals and do not hybridize noticeably.

The second trend in the variation of the electronic structure is connected with an increased distance between the atoms with parallel spins in the case of AFM. If the intrasublattice interactions play the leading role in the formation of the electronic structure the increased interatomic distances lead to the narrowing of the bands.

In the case of unsupported ferromagnetic ML the spin splitting is larger than the band width (Fig. 3). The transition to AFM leads to the narrowing of the bands. There is, however, no noticeable hybridization of the spin-up and spin-down states. Therefore, there is no redistribution of the Fe 3*d* states between local spin-up and spin-down channels. The atomic magnetic moment remains practically unchanged (Table I).

In the case of Fe ML on W(001) the Fe-W hybridization results in much broader bands (Fig. 3). The transition to AFM leads to strong spin hybridization in an energy interval between −0.1 Ry and the Fermi level. One can also notice changes related to the narrowing of the bands. For example, the decrease of the spin-up DOS in the energy interval between −0.13 and −0.1 Ry that makes the spin-up states below −0.1 Ry energetically more compact than in FM. At the same time the number of the spin-down states below −0.1 Ry and the number of the spin-up states above the Fermi energy decrease. The variation in the electronic structure leads to the increase of the magnetic moment while the total number of the 3*d* electrons remains almost unchanged. As the result of these changes the occupied part of the 3*d* states lowers the energy that makes the antiferromagnetism preferable and, therefore, the leading exchange parameters antiferromagnetic. On the other hand, for the unsupported Fe ML the transition to AFM leads to an increase of the energy due to the increased energy of the occupied spin-down states.

These trends reveal themselves also in the frozen-magnon energies since the noncollinearity of the Fe moments gives rise to both spin hybridization and band narrowing. Since the effect increases with increasing angles between nearest moments the trends are better visualized in the DOS of the AFM state.

C. Néel temperature

The mapping of an itinerant-electron system onto Heisenberg Hamiltonian with a subsequent application of a statistical mechanics scheme is a standard tool to study the thermodynamics of itinerant-electron magnets.[8] The knowledge of the Heisenberg exchange parameters is not, however, sufficient for the estimation of the Néel temperature of two-dimensional (2D) antiferromagnets. Indeed, in this case the Mermin-Wagner theorem[12] applies. This theorem states that the isotropic 2D Heisenberg antiferromagnet cannot order above zero temperature since the order is destroyed by the long-wavelength fluctuations. To obtain a nonzero Néel tem-

perature the magnetic anisotropy must be taken into account. An estimation of the magnetic anisotropy that can be used in the calculation of the Néel temperature is given in Ref. 1.

The simplest statistical-mechanics method to estimate the magnetic transition temperature is the mean-field approximation.[8,14] This method is, however, unsatisfactory in the case of 2D magnets since it neglects the long-wavelength fluctuations and, therefore, gives a nonzero value of the magnetic transition temperature for isotropic Heisenberg Hamiltonian contradicting to the Mermin-Wagner theorem.

Much better suited for the study of the 2D systems is the random phase approximation (RPA).[13,14] For the ferromagnetic ground state the formula for the Curie temperature takes the form

$$\frac{1}{k_B T_C^{\mathrm{RPA}}} = \frac{6\mu_B}{M}\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{\omega(\mathbf{q})}, \tag{5}$$

where $\omega(\mathbf{q})$ is the spin-wave dispersion, μ_B is the Bohr magneton, N is the number of $\mathbf{q}$ points in the first Brillouin zone, and M is the atomic magnetic moment.

For an isotropic 2D Heisenberg magnet the sum in the right part becomes singular leading, in agreement with the Mermin-Wagner theorem, to a zero value of the Curie temperature. The magnetic anisotropy Δ produces the gap in the magnon spectrum $[\omega(\mathbf{q}) \rightarrow \omega(\mathbf{q}) + \Delta]$ and leads to nonzero Curie temperature.[15] Here Δ is the magnetic-anisotropy energy per Fe atom. Since the dependence of the Curie temperature on the magnetic anisotropy has weak logarithmic character, an approximate knowledge of the value of the magnetic anisotropy is sufficient to get a good estimation of the Curie temperature.

In the present paper we are dealing with a 2D antiferromagnet and, therefore, Eq. (5) giving the Curie temperature seems to be irrelevant. It can, however, be shown that within the RPA the Néel temperature of a two-sublattice Heisenberg antiferromagnet is equal to the Curie temperature of the Heisenberg ferromagnet obtained by reversing the sign of all intersublattice interactions.[16] This property allows the use of Eq. (5) to determine the Néel temperature.

In Fig. 4 we present the Néel temperature as a function of the anisotropy parameter Δ. The Néel temperature is zero for $\Delta = 0$. For nonzero Δ, there is first a narrow interval of fast increase of the Néel temperature. For larger Δ, the increase becomes rather shallow.[17] The value of $\Delta_{(\mathrm{Fe/W})} = 0.176$ mRy obtained by Kubetzka *et al.*, corresponds to the Néel temperature of about 260 K. For comparison, the magnetic anisotropy of $\frac{1}{2}\Delta_{(\mathrm{Fe/W})}$ gives $T_N = 240$ K while the anisotropy of $2\Delta_{(\mathrm{Fe/W})}$ results in the Néel temperature about 290 K.

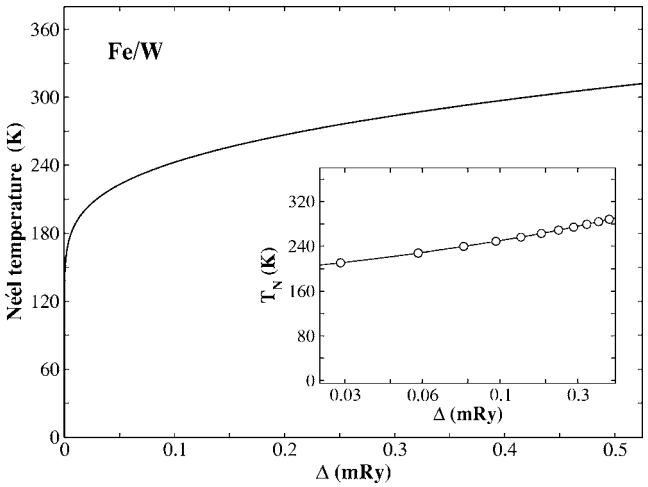

FIG. 4. The Néel temperature of the Fe layer on W(001) as a function of the anisotropy parameter Δ. The inset shows a part of the curve with the use of the logarithmic scale on the abscissa.

IV. CONCLUSIONS

Summarizing we report the study of the properties of Fe ML on W(001) that has been found experimentally to possess a unique in-plane antiferromagnetic structure. We demonstrate that the instability with respect to the formation of the state characterized by wave vector $\mathbf{q} = (1\ 1)$ can be established in the study of the frozen magnon states of the ferromagnetic configuration. We show, however, that there is substantial dependence of the calculated exchange parameters on the reference state. We agree with the conclusion by Ferriani *et al.*, that the Fe-W hybridization plays a crucial role in the formation of the antiferromagnetic structure. Our calculations demonstrate that the Fe-W exchange interaction is much weaker than Fe-Fe interaction. Therefore our scenario of the transition from the ferromagnetism of the unsupported Fe ML to the antiferromagnetism of Fe ML on W(001) consists in the strong variation of the Fe-Fe exchange interactions caused by the change in the electronic structure generated by the Fe-W hybridization. We use the exchange parameters obtained for the ground state antiferromagnetic structure to estimate the value of the Néel temperature.

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