MAGNETIC DOMAIN PINNING AT GRAIN BOUNDARIES

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1. Introduction

Paper describes the essence of interaction between magnetic domains and structural disturbances in the crystal lattice of magnetic materials. Although it is undoubtedly a very interesting issue, detailed investigation and the relationship between the magnetic domain and the structural defect at the microscopic level is still missing [1]. The aim of this article is to clarify this relationship and to find macroscopic explanation. For detailed identification of the problem we have used both, experimental identification using magnetic force microscope (MFM) and simulation methods based on density functional theory (DFT). Both techniques indicate on a high sensitivity of magnetic effect on crystal imperfections in a good agreement. The results could be used for explanation outcome of non-destructive testing of magnetic materials.

2. Theoretical background

Magnetic domain is a macroscopic area where magnetic saturation occurs. Simply put, "all" magnetic spins are oriented in one direction. It is clear that such strong magnetization must be compensated by another region that is naturally magnetized in the opposite direction. Neighboring areas are separated by a dynamic interface that we call Bloch's wall. The width of the wall changes due to the two opposing energies, anisotropy and exchange, that create it, and also as a result of defects placed in the crystal lattice. The first step in our experiment was to identify the existing imperfections in the lattice. For this we used an atomic force microscope (AFM) in configuration for magnetic measurements (MFM), which gave us good information about the distribution of flaws in the area on the surface of the material. In the second step, we performed a scan of the surface in which we identified the magnetic properties. Due to the special function of the used microscope, we were able to identified both scans with high precision. The results show on the interaction between surface defects and boundaries between domains. These results made us happy but the question of why it is so, stayed.

In this case helps numerical simulation. We used the technique based on the DFT. This method makes it possible to estimate the distribution of the magnetic moment in the vicinity of the interface. It is unfortunate, as always, the small number of atoms that we can include in the calculation. So as usual we have to be satisfied with the estimates but after long-term calculations, we have confirmed experimental observations. We did not mind working because it was a massive parallel computer which did effort. The details of both experiments are described in details in following part. So, do not despair and read the next part.

3. Experimental details

The MFM measurements were performed on steel specimen referred as XT8. The composition of the XT8 sample is shown in Table 1. Since the surface cleanliness is important in this type of experiment, special attention has been devoted to surface preparation. Namely, the surface was etched in HCl acid. The acid was mixed with water in ratio of 1:15 and applied in two steps. The sample was first immersed in the acid for 2 minutes and then checked on optical microscope. After that it was immersed again into the acid for the time of 5 more minutes. After that MFM measurements in Tapping & Lift mode with probe MESP were performed. Various scan sizes were investigated, 1x1 μm, 3x3 μm and 20x20 μm. Height and phase profile of 3x3 μm MFM scan is showed in Figure 1. Height scan represents grain structure and phase profile magnetic domain structure. The 3D imagination of grain and phase profile overlap is shown in Figure 2. After detailed analysis, it can be seen, that change of magnetic profile follows valleys created by grain profile. This analysis can be considered as experimental evidence of magnetic domain pinning at grain boundaries.

Tab. 1. *Composition of the steel sample XT8 used for MFM experiment*

XT8	Fe	C	Si	Mn	Mo	Ni	Cr	Cu	P	S	V	Co
%	94.769	0.18	0.24	0.52	0.62	1.26	2.22	0.08	0.01	0.013	0.08	0.008

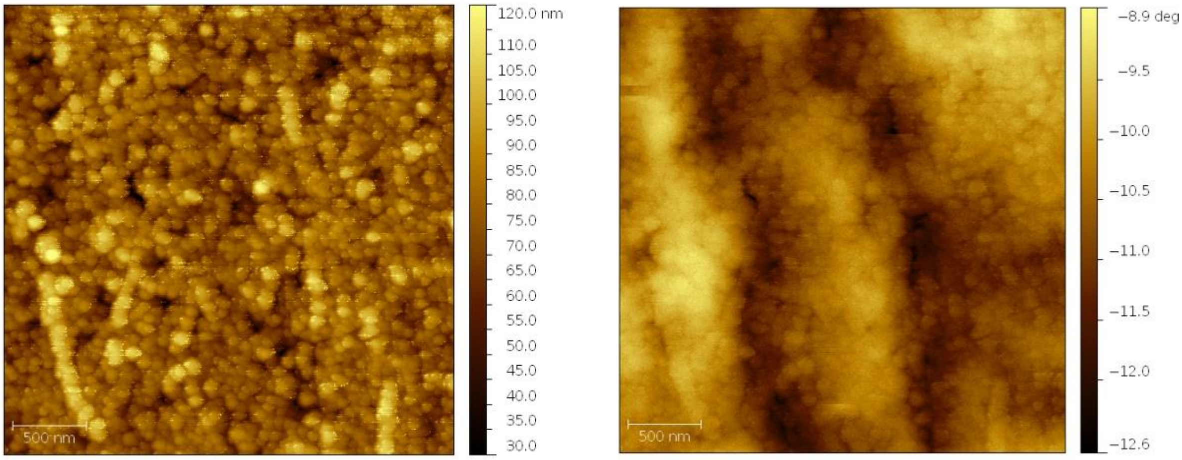

Fig.1: MFM scan, (3x3)μm, height profile (left panel) and phase profile (right panel). Surface and magnetic measurements were made in two different scans using a very accurate navigation of the measuring tip. (colour online)

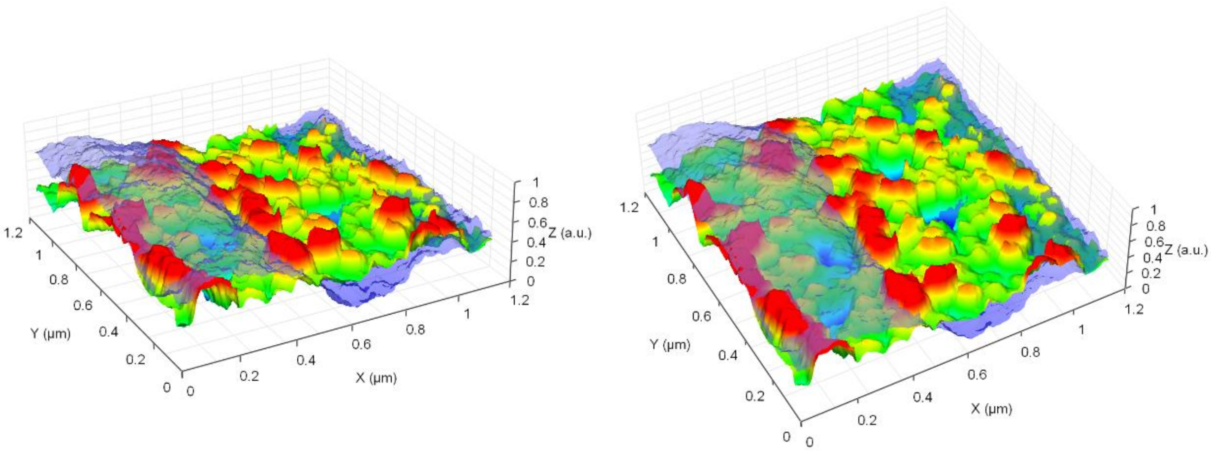

Fig.2: *3D imagination of height profile representing grain structure (red-green) and phase profile representing domain structure (blue). Two different views. The interaction between grain structure and magnetic domain is well observable. (colour online)*

4. Numerical experiment

We have created a model interface that simulates a crystal imperfection. Due to the complications in calculation we have to limit to 100 atoms, which is far from real situation. However, as an explanation of trends this will be enough. Model interface was created using the fact that a special superposition of two periodic lattices can produce real grain boundary (GB) pattern of various types [2]. The type of GB is given by an angle which is kept between the lattices. In this experiment has been used a set of special angles which give tilt grain boundaries Σ5(210), Σ5(310), Σ17(410) and Σ13(510). The geometry optimization, which is in the general a very difficult problem, has been done by very powerful technique combining simulated annealing with genetic algorithm.

Using complicated calculations made by our parallel computer, we were able to calculate local magnetization in the interface. We have used the DFT method and paid attention to all standard convergence tests. In the case of magnetic calculations, it is necessary to pay increased attention to these tests, in order to predict the disappointment after a long computation. The inverse k-space was sampled by 2x2x2 pattern and electron distribution was decomposed into plane waves which we cut off at 1632 eV. To ensure that passports are correctly set, we used Fermi-Dirac smearing 0.27 eV. Higher energy in the smearing of the bands could interfere with the spin distribution right up and down. These results were then transferred to the atomic cluster and in graphical form we showed them in Figure 3. The results were remarkably and fully confirmed by experimental results. For more please read the following part. Details how we design interfaces and more detailed analysis of local magnetic behavior on GB can be found in paper [3].

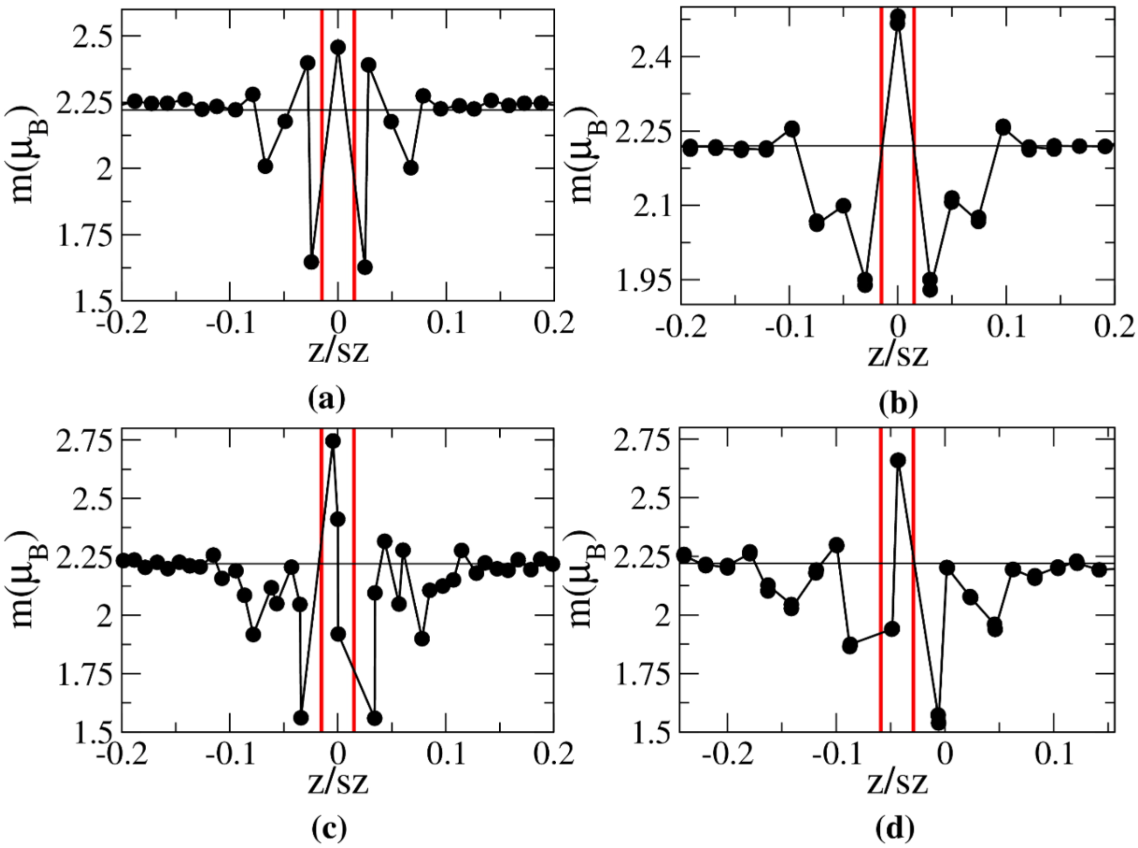

Fig.3: *Variation of local magnetic moments of Fe atoms at GBs (a) Σ5(210), (b) Σ5(310), (c) Σ17(410), (d) Σ13(510). The positions of atoms are presented with respect to the supercell size (sz). Experimental bulk magnetic moment value 2.22 μB is indicated by horizontal solid line and GB plane is positioned between two vertical lines.* [3]

5. Summary

The results of our study are very encouraging. Let's take a look at Figure 2, which shows in a cross-sectional form the relationship between lattice disturbances and magnetic domains. Interaction between the damaged area and the magnetic wall is well visible. From macroscopic looks, this effect is demonstrated through the Barkhausen noise, and is often used in practice.

This phenomenon is interpreted as capturing the walls of magnetic domains into cracks in materials, and this explanation has been widely accepted, although it does not make much sense. Our numerical experiments have shown that the grabbing of the wall takes place through changes in the magnetic moment located on the grid fault. The change of magnetic moment is very precisely localized and bound on a volume to one atom. This parameter is very sensitive to the type of interface (see Fig. 3), so it will be possible to determine not only the concentration of defects but also the type of interface by study of Barkhausen's noise in the future.

Overall, it can be said that the existence of high-tech experimental equipment at a reasonable price and the advent of highly-performing computers and their optimal connection in a high-quality experiment will bring fruit that we will use in technical practice. It could be noted that another useful application of the effect of interaction between imperfections and magnetic domains is to embrace highly powerful magnetic memory which in sure deserve increased attention [4].

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