MOLECULAR PHYSICS REPORTS **40** (2004) 172-175

SIZE DEPENDENCE OF T_C IN Ni THIN FILMS AND NANOWIRES. THE PROBLEM OF RANGE OF INTERACTIONS

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Abstract. A simple model has been proposed by Zhang and Willis to explain the finite size scaling ruling the thickness dependence of the experimental values of the Curie temperature of thin Ni films. It based on an assumption that the range of exchange interaction in Ni metal covers several interatomic distances, thus defining the number of neighbours interacting with a central spin, and hence the Curie temperature T_C in an effective field approximation. The absence of certain neighbours outside the film leads to $T_C(n)$ reduced with respect to that valid for a bulk body the more the thinner is the film. A similar behaviour has been observed in Ni nanowires. We have found that a straightforward calculation applying the same method to wires investigated by Sun *et al*. leads to an exchange interaction range much different from that previously found for Ni in bulk and film forms. This disagreement calls for a further analysis.

1. INTRODUCTION

Recently, wires of nanometer sizes made of nickel [1] have been obtained. Investigations of physical properties, and in particular magnetic transition temperature [1] in these newly available systems are of interest from the point of view of fundamental knowledge as well as applications.

A simple model has been proposed by Zhang and Willis to explain the finite size scaling ruling the thickness dependence of the experimental values of the Curie temperature of thin Ni films. Their approach has lead, in the case of films, to a range of interactions of about 5 distances between consecutive atom layers, *e.g.*, about 10 Å for Ni(111).

We shall show that the same approach applied to Ni nanowires (cf. Ref. [1] for the experimental data) leads to a different range of Ni-Ni interactions. We shall calculate $T_C(d)$ (cf. Ref. [1]) as dependent on the diameter d of Ni nanowire within the simple approach of Zhang and Willis [2]. We shall focus on the problem of the range $R = N_0 a$ of Ni-Ni interactions in the nanowires. Following Zhang and Willis, we assume a model in which spins on a lattice sites are coupled to a cluster of such spins within the range of interaction aN_0, where a is the distance between the consecutive atomic layers and $2aN_0$ is the size of the cluster. Within this approximation, the Curie temperature

$$T_C = k_B^{-1} JN,$$

where N is the number of pairwise interactions and J is the spin-spin coupling energy constant. We admit the uniform magnetization directed along the axis of the wire throughout this work.

2. SQUARE CROSS-SECTION NANOWIRES – COUNTING THE INTERACTING NEIGHBOURS

The cross-sections of the wires in the Sun *et al.* experiment [1] were of diamond shape. For simplicity sake we shall consider the nanowires with square cross sections with sides of length na. Henceforth, we shall omit the factor a unless necessary. Note that the method assumes counting the interacting neighbours of a spin within the "cluster size equivalent to a cube of side $2N_0$" [2]. We have checked that replacing the putative sphere of interactions by a cube does not affect the results essentially, but simplifies the counting.

2. 1. Interactions in a film

It is instructive to repeat first the calculation for the thin film due to Zhang and Willis. The crossed parts in Fig. 1 representing the spins at the faces of the film contain those spins with lacking some neighbours within the range of interaction N_0. The central spin of a cluster lying

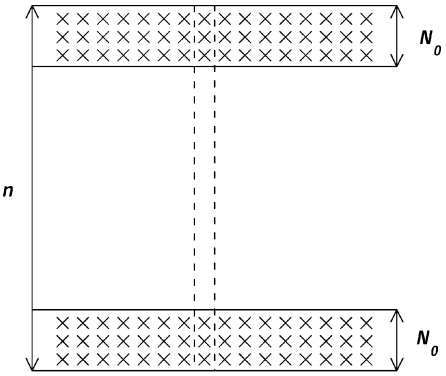

Fig. 1. Thin film scheme showing regions (areas filled with crosses ×) affected by a lack of some neighbours within the range of interaction N_0

within the i-th atomic layer from each surface (starting with $i = 0$ at the surface) loses (N_0, i) $(2N_0)^2$ interactions with respect to that embedded in the bulk. Since

$$\sum_{i=0}^{N_0-1}\left(N_0-i\right)\left(2N_0\right)^2=\frac{1}{2}N_0\left(N_0+1\right)\left(2N_0\right)^2, \tag{2}$$

the number of pairwise interactions in each column of spins (perpendicular to the surface and marked by dashed lines in Fig. 1) within the film of thickness n reduces by $N_0(N_0 + 1)(2N_0)^2$ to give altogether

$$n\left(2N_0\right)^3-N_0\left(N_0+1\right)\left(2N_0\right)^2 \tag{3}$$

leading to

$$1-\frac{T_C(n)}{T_C}=\frac{\left(N_0+1\right)}{2n} \qquad (n>N_0). \tag{4}$$

2.2. Interactions in a wire

Let us limit ourselves to $N_0 < n$ merely because such is the experimental situation we are dealing with. Hence, within the range N_0 are all spins filling a sphere of the radius N_0, or, approximately, those filling a cube of the edge $2N_0$. For a wire embedded in the bulk, the number of pairwise interactions of a given spin is $n^2(2N_0)^3$. The spins in the wire of a square cross section shall be divided into several parts. The first part consists of such spins (marked with crosses × in Fig. 2) that have no edge spins within their range of interaction and yet do have such spins on one of the faces of the wire. The next part comprises such spins interacting with the edge spins (marked with full symbols • in Fig. 2). The rest consists of spins with bulk-type neighbourhood.

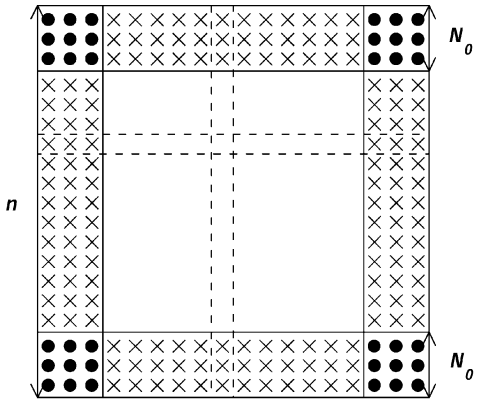

Fig. 2. Wire cross-section scheme showing regions affected by a lack of some neighbours within the range of interaction N_0 due to the presence of one surface (areas filled with crosses ×) or due to the presence of two adjacent faces of the wire (areas filled with full symbols •)

We obtain $N_0(N_0 + 1)(2N_0)^2$ per column of lacking neighbours of the spins × of the first group. Yet there are $n \cdot 2N_0$ such horizontal and the same number of perpendicular columns (marked by dashed lines) per cross section as illustrated in Fig. 2. Hence, these "film-like" contributions to the sum of lacking interactions give altogether $2(n \cdot 2N_0)(N_0 + 1)(2N_0)^3$.

It remains to subtract the wire edge (or cross section corner) terms yet. A spin in the corner of the square cross section of the wire lacks $(3/4)(2N_0)^3 = 6(N_0)^3$ interactions with respect to the bulk. In general, a spin within the edge area (marked with full symbols • in Fig. 2) having discrete coordinates i and j with respect to the faces of the wire (edges of the square) lacks $(N_0 - i)(N_0 - j)(2N_0) + (N_0 + i)(N_0 - j)(2N_0) + (N_0 - i)(N_0 + j)(2N_0) = 6(N_0)^3 - 2(i + j)(N_0)^2 + 2ijN_0$ interactions with respect to the bulk. Summing up over i and j from 0 to $N_0 - 1$ for each edge area and taking into account that there are four such areas, one obtains the edges contribution $N_0^3(30 - 4N_0 - 2N_0^2)$. Hence,

$$1 - \frac{T_C(d)}{T_C} = 1 - \frac{T_C(n)}{T_C} = \frac{N_0 + 1}{n} - \frac{9N_0^2 + 10N_0 - 15}{4n^2}. \tag{5}$$

3. RESULTS AND DISCUSSION

Plotting the experimental data of $T_C(d)$ as a function of the wire diameter $d = na$ taken from Ref. [1] (full symbols • in Fig. 3), and fitting Eq. (5) to the data with $R = N_0 a$ as a parameter, we obtain the fit presented in Fig. 3 as a line. The best fit is obtained for $R = 22.4$ Å. Note that the thinnest Ni wires investigated up to now [1] are thicker than the thickest films investigated in Ref. [2]. Zhang and Willis [2] discussed the same experimental data by Sun et al. [1] suggesting that the rapid drop of the T_C occurring at much larger thicknesses in the wires "is simply due to the increased surface/volume ratio in the nanowires

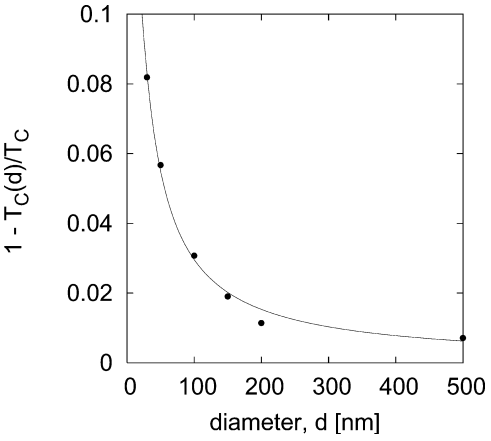

Fig. 3. The shift $[T_C - T_C(d)]/T_C$ of the Curie temperature $T_C(d)$ of Ni nanowires of diameter d with respect to the bulk value T_C, plotted as a function of the diameter d. The full symbols mark the selected experimental data taken from Ref. [1]. The line represents the best fit of Eq. (5) to the data with the effective range aN_0 of spin-spin interactions as a parameter

compare to the thin films for the same thickness" [2]. We have confirmed that this is qualitatively indeed the case, as seen from our Eq. (5) and the corresponding Fig. 3. However, quantitatively the ranges of spin-spin interactions differ a lot ($R = 22.4$ Å for the wires *vs. ca* 6-10 Å for the films, depending on their orientation). It is hard to accept physically. This suggests to raise a question about the limits of applicability of the Zhang and Willis method. A possible way out lies perhaps in a properly modified scaling approach.

Acknowledgments

The work of one of us (ARF) was supported by Grant No. PO3B 120 23 of the Polish Committee for Scientific Research.

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