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Addition/Correction

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Correction to "Ab Initio Study of the Structural, Electronic, Magnetic, and Hyperfine Properties of $Ga_xFe_{4-x}N$ ($0.00 \leq x \leq 1.00$) Nitrides"

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In the previous published paper, ref 1, about the variation of the structural, magnetic, and hyperfine properties of $Ga_xFe_{4-x}N$ with the concentration of Ga (x), we have used ab initio calculations based on the density functional theory (DFT). We arrived at the conclusion that the ternary compounds studied show a nonlinear increasing of the lattice parameter (a) with x. This behavior is supported with experimental data obtained using a powder diffractometer with Cu $K\alpha_1$ radiation,[2] whereas measurements using Mo $K\alpha_1$ radiation[3] show a different behavior.

In ref 1, we have considered the experimental data from ref 2 because a known value of the lattice constant (a) of γ'-Fe_4N is reported, which is our starting compound. In ref 3, an overestimate of the a value shows differences with other experimental values where either Cu $K\alpha_1$[4,5] or Mo $K\alpha_1$[6] radiation was used.

Regrettably, in figure 3 of ref 1, we made a mistake in the transcription of x values that has been observed and commented by R. Dronskowski.[7] We have corrected figure 3 of ref 1 by figure 1, where we have found a similar behavior of a with respect to x. So, fitting this experimental data (intended composition) with a similar equation described in ref 1, we found eq 1 that is in agreement with theoretical data fit.[1] Furthermore, for comparison, we have added the experimental data from ref 3 to Figure 1.

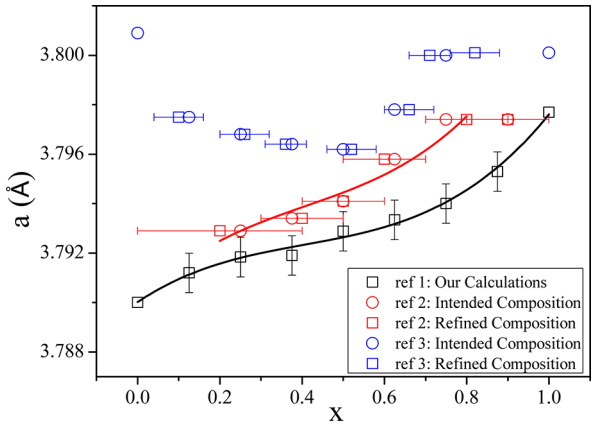

Figure 1. Variation of a with x from ab initio calculation and experimental data.

$$a^{exp}(x) = 3.7900_2(1 - x) + 3.8020_3x + 0.0051_5x(1 - x)^2 - 0.0175_6x^2(1 - x) \quad (1)$$

In refs 2 and 3, by simplicity the authors denominated the compounds $Ga_{0.9}Fe_{3.1}N$ and $Ga_{0.82}Fe_{3.18}N$, respectively, as $GaFe_3N$, and suggest that these materials could be an antiferromagnetic compound. Because the measured moment of these is clearly above zero,[2,3] we prefer to call this system a ferrimagnetic compound. Furthermore, in figure 7 in ref 1, we have included a wrong experimental point of M_{fu} belonging to x = 1; this value has not been reported in ref 2.

We accept the genuine errors pointed out by R. Dronskowski,[7] and we are very grateful to him, but we believe in our studies on $Ga_xFe_{4-x}N$ and $GaFe_3N$ and affirm that the results are correct according to our calculations and we support our results previously published with enough amount of data. This is the reason why we have presented this communication as an erratum to ref 1 as well as a complement to our theoretical perspective of ref 1.

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