Data Article

Modelling data for Predicting New Iron Garnet Thin Films with Perpendicular Magnetic Anisotropy

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ABSTRACT

These data include detailed calculations and graphs based on our manuscript submitted to Journal of Magnetism and Magnetic Materials, entitled “Predicting New Iron Garnet Thin Films with Perpendicular Magnetic Anisotropy”. These data are organized in two parts; first, we present the calculated plots of sensitivity of magnetic anisotropy field and anisotropy energy density for 49 epitaxial rare earth iron garnet (REIG) film/substrate pairs (a total of 98 plots, Figs. 1–15). In the second part, we present in Table 1 the complete details on the calculations for total magnetic anisotropy and all material constants used for each of 50 film/substrate pairs. The comparison with the previous experimental demonstrations is also shown in Table 1 (last column) and 2 with an accompanying discussion confirming the reliability of our model.

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1. Data

This data article provides a detailed calculation of effective magnetic anisotropy energy density of 50 different rare earth iron garnet/substrate pairs. Figs. 1–15 demonstrate the sensitivity of total magnetic anisotropy energy density (left column) and magnetic anisotropy field (right column) on strain and saturation magnetization variabilities. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, are shown for Fig. 1. (a) and (b) YIG, (c) and (d) TmIG, (e) and
(f) DyIG. Fig. 2. (a) and (b) HoIG, (c) and (d) ErIG, (e) and (f) YbIG, and Fig. 3. (a) and (b) TblIG, (c) and (d) GdIG, (e) and (f) SmIG, (g) and (h) EuIG grown on GGG substrate. In addition, Fig. 4(a–f), Fig. 5(a–f) and Fig. 6(a–h) show the change of $K_{\text{eff}}$ and $H_a$ with $M_s$ and strain of YIG, TmIG, DyIG, HoIG, ErIG, YbIG, TblIG, GdIG, SmIG, and EuIG thin films grown on YAG. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) YIG, (c) and (d) TmIG, (e) and (f) DyIG grown on GGG substrate.

Fig. 1. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) YIG, (c) and (d) TmIG, (e) and (f) DyIG grown on GGG substrate. S.M. Zanjani, M.C. Onbaslı / Data in brief 28 (2020) 104937

Table 1 shows the theoretical, measured and calculated parameters of effective magnetic anisotropy energy density ($K_{\text{eff}}$). Table 2 includes the comparison of magnetic anisotropy state predicted by our model with previous experimental demonstrations.
2. Experimental design, materials and methods

2.1. Analytical calculation method of magnetic anisotropy energy density and field

In order to calculate the effective anisotropy energy density we used $K_{\text{eff}} = K_{\text{indu}} + K_{\text{shape}} + K_1$ equation to calculate the total anisotropy energy density for 50 thin film rare earth iron garnet/substrate pairs. Figs. 1–15 exclude the Gadolinium Iron Garnet (GdIG) film on substituted Gadolinium Gallium Garnet (SGGG) substrate because there is no lattice mismatch between the film and the substrate. Each anisotropy term consist of the following parameters: $K_{\text{eff}} = -\frac{3111111111111}{2\pi^2} \sigma^{\parallel} + 2\pi M_s^2 + K_1$. The energy

Fig. 2. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) HoIG, (c) and (d) ErIG, (e) and (f) YbIG grown on GGG substrate.
Fig. 3. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) TbIG, (c) and (d) GdIG, (e) and (f) SmIG, (g) and (h) EuIG grown on GGG substrate.
density was calculated based on the parameters reported in previous references [1–6] and calculated terms according to their formulae (i.e. $\varepsilon_{ij} = \frac{a_{sub}}{C_0 a_{film}}$). First-order magnetocrystalline anisotropy, $K_1$, is an intrinsic temperature-dependent constant reported for each REIG material. Young’s modulus ($Y$), Poisson’s ratio ($\nu$) and magnetostriction constant ($\lambda_{111}$) parameters evolving in the magnetoelastic anisotropy energy density term (first term) are considered to be constant according to the values previously reported. For shape anisotropy energy calculations (second term), bulk saturation magnetization ($M_s$) for each film was used. Since each film may exhibit variability in $M_s$ with respect to bulk, the model presented here yields the most accurate predictions when the experimental film $M_s, \lambda_{111}, Y, \nu$ and $K_1$, and in-plane strain values are entered for each term. Table 1 shows the theoretical, measured and calculated parameters of anisotropy energy density terms and contributing parameters. In Table 2, we present a comparison of our model’s predictions with the previous experimental studies. Anisotropy

![Fig. 4. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) YIG, (c) and (d) TmIG, (e) and (f) DyIG grown on YAG substrate.](image-url)
fields were calculated using \( H_a = 2 \frac{K_{eff}}{M_s} \) formula. The original Microsoft Excel and MATLAB files used for generating the data for Figs. 1–15 are also presented.

2.2. Predictive capability and validity of our model

We tested the prediction accuracy of our model by going through each available experimental demonstration of garnet thin film/substrate anisotropy characterization and comparing their measured anisotropy with the predictions of our model. Below, we show the prediction accuracy and cases where experiments are different from our predictions.

As shown in the table above, our model is able to predict the magnetic anisotropy state of almost all garnet/substrate combinations.
Fig. 6. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) TbIG, (c) and (d) GdIG, (e) and (f) SmIG, (g) and (h) EuIG grown on YAG substrate.
Fig. 7. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) YIG, (c) and (d) TmIG, (e) and (f) DyIG grown on SGGG substrate.
Fig. 8. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) HoIG, (c) and (d) ErIG, (e) and (f) YbIG grown on SGGG substrate.
Fig. 9. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) TbIG, (c) and (d) SmIG, (e) and (f) EuIG grown on SGGG substrate.
Fig. 10. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) YIG, (c) and (d) TmIG, (e) and (f) DyIG grown on TGG substrate.
Fig. 11. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) HoIG, (c) and (d) ErIG, (e) and (f) YbIG grown on TGG substrate.
Fig. 12. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) TbIG, (c) and (d) GdIG, (e) and (f) SmIG, (g) and (h) EuIG grown on TGG substrate.
Fig. 13. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective
anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field,
respectively, for (a) and (b) YIG, (c) and (d) TmIG, (e) and (f) DyIG grown on NGG substrate.
Fig. 14. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) HoIG, (c) and (d) ErIG, (e) and (f) YbIG grown on NGG substrate.
Fig. 15. Effect of partial film relaxation or additional strain and saturation magnetic moment variability on the film effective anisotropy energy density and anisotropy field. Variation of effective magnetic anisotropy energy density and anisotropy field, respectively, for (a) and (b) TbIG, (c) and (d) GdIG, (e) and (f) SmIG, (g) and (h) EuIG grown on NGG substrate.
| RIG | \( M_r \) (kA m\(^{-1}\)) | \( K_{\text{shape}} \) (erg cm\(^{-3}\)) | \( a_{||} \) (Å) | \( \epsilon_|| \) | \( \sigma_{ij} \) (dyn cm\(^{-2}\)) | \( \lambda_{111} \) | \( K_{\text{incl}} \) (erg cm\(^{-3}\)) | \( K_I \) (300K) (erg cm\(^{-3}\)) | \( K_{\text{eff}} \) (erg cm\(^{-3}\)) | Experimental Demonstration |
|-----|----------------|-----------------|-----------|--------|----------------|--------|----------------|----------------|----------------|----------------|
| YIG | 141.7 | 1.26 \( \times \) 10\(^5\) | 12376 | 5.66 \( \times \) 10\(^{-4}\) | 1.59 \( \times \) 10\(^3\) | \(-2.40 \times 10^{-6}\) | 5.74 \( \times \) 10\(^3\) | \(-6.10 \times 10^{3}\) | 1.26 \( \times \) 10\(^5\) | [7] (Bi-Doped) |
| TmIG | 110.9 | 7.72 \( \times \) 10\(^4\) | 12324 | 4.79 \( \times \) 10\(^{-3}\) | 1.35 \( \times \) 10\(^{10}\) | \(-5.20 \times 10^{-6}\) | 1.05 \( \times \) 10\(^3\) | \(-5.80 \times 10^{3}\) | 1.77 \( \times \) 10\(^5\) | [8] (doped stoichiometry) |
| DyIG | 31.8 | 6.37 \( \times \) 10\(^3\) | 1244 | \(-4.58 \times 10^{-3}\) | \(-1.29 \times 10^{10}\) | \(-5.90 \times 10^{-6}\) | \(-1.14E \times 10^{5}\) | \(-5.00 \times 10^{3}\) | \(-1.13 \times 10^{5}\) | |
| HoIG | 55.7 | 1.95 \( \times \) 10\(^4\) | 124 | \(-1.37 \times 10^{-3}\) | \(-3.86 \times 10^{9}\) | \(-4.00 \times 10^{-6}\) | \(-2.32 \times 10^{4}\) | \(-5.00 \times 10^{3}\) | \(-8.66 \times 10^{4}\) | [9] |
| ErIG | 79.6 | 3.98 \( \times \) 10\(^4\) | 1235 | 2.67 \( \times \) 10\(^{-3}\) | 7.53 \( \times \) 10\(^9\) | \(-4.90 \times 10^{-6}\) | 5.53 \( \times \) 10\(^4\) | \(-6.00 \times 10^{3}\) | 8.91 \( \times \) 10\(^4\) | |
| YbIG | 127.4 | 1.02 \( \times \) 10\(^5\) | 123 | 6.75 \( \times \) 10\(^{-3}\) | 1.90 \( \times \) 10\(^{10}\) | \(-4.50 \times 10^{-6}\) | 1.28 \( \times \) 10\(^5\) | \(-6.10 \times 10^{3}\) | 2.24 \( \times \) 10\(^5\) | |
| TbIG | 15.9 | 1.59 \( \times \) 10\(^3\) | 1246 | \(-6.18 \times 10^{-3}\) | \(-1.74 \times 10^{10}\) | 1.20 \( \times \) 10\(^{-5}\) | 3.13 \( \times \) 10\(^5\) | \(-8.20 \times 10^{3}\) | 3.07 \( \times \) 10\(^5\) | |
| GdIG | 7.9 | 3.98 \( \times \) 10\(^2\) | 1248 | \(-7.77 \times 10^{-3}\) | \(-2.19 \times 10^{10}\) | \(-3.10 \times 10^{-6}\) | \(-1.02 \times 10^{5}\) | \(-4.10 \times 10^{3}\) | \(-1.06 \times 10^{5}\) | [10] |
| SmIG | 140 | 1.23 \( \times \) 10\(^5\) | 1253 | \(-1.17 \times 10^{-2}\) | \(-3.30 \times 10^{10}\) | \(-8.60 \times 10^{-6}\) | \(-4.26 \times 10^{5}\) | \(-1.74 \times 10^{5}\) | \(-3.21 \times 10^{5}\) | [11] |
| EuIG | 92.1 | 5.33 \( \times \) 10\(^4\) | 125 | \(-1.30 \times 10^{-2}\) | \(-3.65 \times 10^{10}\) | 1.80 \( \times \) 10\(^{-8}\) | 9.86 \( \times \) 10\(^3\) | \(-3.80 \times 10^{3}\) | 1.14 \( \times \) 10\(^5\) | [12] (PMA on GGG (001)) |

**Table 1**
Calculation of contributing terms to effective magnetic anisotropy energy density \( K_{\text{eff}} \).
|     | $a_{\text{NGG}}$ |     |     |     |     |     |     |     |
|-----|-----------------|-----|-----|-----|-----|-----|-----|-----|
| DyIG | 31.847          | $6.37 \times 10^3$ | 12.44 | $-6.83 \times 10^{-3}$ | $-1.92 \times 10^{10}$ | $-5.90 \times 10^{-6}$ | $-1.70 \times 10^5$ | $-5.00 \times 10^4$ | $-1.69 \times 10^5$ |
| HoIG | 55.732          | $1.95 \times 10^4$ | 12.4 | $-3.63 \times 10^{-3}$ | $-1.02 \times 10^{10}$ | $-4.00 \times 10^{-6}$ | $-6.13 \times 10^4$ | $-5.00 \times 10^4$ | $-4.68 \times 10^4$ |
| ErIG | 79.618          | $3.98 \times 10^4$ | 12.35 | $4.05 \times 10^{-4}$ | $1.14 \times 10^9$ | $-4.90 \times 10^{-6}$ | $8.38 \times 10^3$ | $-6.00 \times 10^3$ | $4.22 \times 10^4$ |
| YbIG | 127.389         | $1.02 \times 10^5$ | 12.3 | $4.47 \times 10^{-3}$ | $1.26 \times 10^{10}$ | $-4.50 \times 10^{-6}$ | $8.50 \times 10^4$ | $-6.10 \times 10^4$ | $1.81 \times 10^5$ |
| TbIG | 15.924          | $1.59 \times 10^3$ | 12.46 | $-8.43 \times 10^{-3}$ | $-2.37 \times 10^{10}$ | $1.20 \times 10^{-5}$ | $4.27 \times 10^5$ | $-8.20 \times 10^4$ | $4.21 \times 10^5$ |
| GdIG | 7.962           | $3.98 \times 10^2$ | 12.48 | $-1.00 \times 10^{-2}$ | $-2.82 \times 10^{10}$ | $-3.10 \times 10^{-6}$ | $-1.31 \times 10^5$ | $-4.10 \times 10^4$ | $-1.35 \times 10^5$ |
| SmIG | 140             | $1.23 \times 10^5$ | 12.53 | $-1.40 \times 10^{-2}$ | $-3.93 \times 10^{10}$ | $-8.60 \times 10^{-6}$ | $-5.08 \times 10^3$ | $-1.74 \times 10^4$ | $-4.02 \times 10^4$ |
| EuIG | 92.1            | $5.33 \times 10^4$ | 12.5 | $-1.32 \times 10^{-2}$ | $-3.72 \times 10^{10}$ | $1.80 \times 10^{-6}$ | $1.00 \times 10^6$ | $-3.80 \times 10^4$ | $1.50 \times 10^5$ |

$\text{aNGG} = 12.509 \, \text{Å}$

YIG: 110.908 | $7.72 \times 10^4$ | 12.324 | $1.50 \times 10^{-2}$ | $4.23 \times 10^{10}$ | $-5.20 \times 10^{-6}$ | $3.30 \times 10^5$ | $-5.80 \times 10^3$ | $4.01 \times 10^5$ |

TmIG: 110.908 | $7.72 \times 10^4$ | 12.324 | $1.50 \times 10^{-2}$ | $4.23 \times 10^{10}$ | $-5.20 \times 10^{-6}$ | $3.30 \times 10^5$ | $-5.80 \times 10^3$ | $4.01 \times 10^5$ |

SmIG: 140 | $1.23 \times 10^5$ | 12.53 | $-1.68 \times 10^{-3}$ | $-4.72 \times 10^{10}$ | $-8.60 \times 10^{-6}$ | $-6.09 \times 10^3$ | $-1.74 \times 10^4$ | $4.48 \times 10^4$ |

EuIG: 92.1 | $5.33 \times 10^4$ | 12.5 | $7.20 \times 10^{-4}$ | $2.03 \times 10^{10}$ | $1.80 \times 10^{-6}$ | $5.48 \times 10^3$ | $-3.80 \times 10^4$ | $4.40 \times 10^4$ |

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Table 2
Comparison of experimental demonstrations of magnetic anisotropy and our model predictions (IP: in-plane, OP: out-of-plane, NA: Not Available).

| No. | Thin Film-Substrate combination | Predicted anisotropy | Published Experimental Studies | Does our prediction match the experiment? | Model does not take into consideration: |
|-----|---------------------------------|----------------------|-------------------------------|------------------------------------------|-----------------------------------------|
| 1   | YIG/GGG                          | IP                   | [13]                          | YES                                      |                                         |
| 2   | TmIG/GGG                         | IP                   | [16]                          | NO                                       | Off-stoichiometry                       |
| 3   | DyIG/GGG                         | OP                   | [8] (doped stoichiometry)     | YES                                      |                                         |
| 4   | HoIG/GGG                         | OP                   | [9]                           | YES                                      |                                         |
| 5   | ErIG/GGG                         | IP                   | [17] - not thin film          | YES                                      |                                         |
| 6   | YbIG/GGG                         | IP                   | NA                            |                                          |                                         |
| 7   | TbIG/GGG                         | IP                   | [15]                          | NO                                       | Ref. [15] contains significant shear stress and reduced ME anisotropy. Off-stoichiometry changes the assumed $M_s, K_1$ and $\lambda_{111}$. |
| 8   | GdIG/GGG                         | OP                   | [10]                          | YES                                      |                                         |
| 9   | SmIG/GGG                         | OP                   | [11]                          | YES                                      |                                         |
| 10  | EuIG/GGG                         | IP                   | [15]                          | NO                                       | Ref. [15] contains significant shear stress and reduced ME anisotropy. Off-stoichiometry changes the assumed $M_s, K_1$ and $\lambda_{111}$. |
| 11  | YIG/YAG                          | OP                   | NA                            |                                          |                                         |
| 12  | TmIG/YAG                         | OP                   | NA                            |                                          |                                         |
| 13  | DyIG/YAG                         | OP                   | NA                            |                                          |                                         |
| 14  | HoIG/YAG                         | OP                   | NA                            |                                          |                                         |
| 15  | ErIG/YAG                         | OP                   | NA                            |                                          |                                         |
| 16  | YbIG/YAG                         | OP                   | NA                            |                                          |                                         |
| 17  | TbIG/YAG                         | IP                   | NA                            |                                          |                                         |
| 18  | GdIG/YAG                         | OP                   | NA                            |                                          |                                         |
| 19  | SmIG/YAG                         | OP                   | NA                            |                                          |                                         |
| 20  | EuIG/YAG                         | IP                   | NA                            |                                          |                                         |
| 21  | YIG/SGGG                         | IP                   | [13]                          | NO                                       | Larger $\lambda_{111}$, strain and $M_s$ used in ref. [13] |
| 22  | TmIG/SGGG                        | IP                   | [14]                          | NO                                       | Off-stoichiometry                       |
| 23  | DyIG/SGGG                        | IP                   | NA                            |                                          |                                         |
| 24  | HoIG/SGGG                        | IP                   | NA                            |                                          |                                         |
| 25  | ErIG/SGGG                        | IP                   | NA                            |                                          |                                         |
| 26  | YbIG/SGGG                        | IP                   | NA                            |                                          |                                         |
| 27  | TbIG/SGGG                        | OP                   | [15]                          | NO                                       | Ref. [15] contains significant shear stress and reduced ME anisotropy. Off-stoichiometry changes the assumed $M_s, K_1$ and $\lambda_{111}$. |
| 28  | GdIG/SGGG                        | OP                   | NA                            |                                          |                                         |
| 29  | SmIG/SGGG                        | OP                   | NA                            |                                          |                                         |
| 30  | EuIG/SGGG                        | IP                   | NA                            |                                          |                                         |
| 31  | YIG/TGG                          | IP                   | NA                            |                                          |                                         |
| 32  | TmIG/TGG                         | IP                   | NA                            |                                          |                                         |
| 33  | DyIG/TGG                         | OP                   | NA                            |                                          |                                         |
| 34  | HoIG/TGG                         | OP                   | NA                            |                                          |                                         |
| 35  | ErIG/TGG                         | IP                   | NA                            |                                          |                                         |
| 36  | YbIG/TGG                         | IP                   | NA                            |                                          |                                         |
| 37  | TbIG/TGG                         | IP                   | NA                            |                                          |                                         |
| 38  | GdIG/TGG                         | OP                   | NA                            |                                          |                                         |
| 39  | SmIG/TGG                         | OP                   | NA                            |                                          |                                         |
| 40  | EuIG/TGG                         | IP                   | NA                            |                                          |                                         |
| 41  | YIG/NGG                          | IP                   | [13]                          | NO                                       | Larger $\lambda_{111}$, strain and $M_s$ used in ref. [13] |
| 42  | TmIG/NGG                         | IP                   | NA                            |                                          |                                         |
| 43  | DyIG/NGG                         | IP                   | NA                            |                                          |                                         |
| 44  | HoIG/NGG                         | IP                   | NA                            |                                          |                                         |
| 45  | ErIG/NGG                         | IP                   | NA                            |                                          |                                         |
| 46  | YbIG/NGG                         | IP                   | NA                            |                                          |                                         |
| 47  | TbIG/NGG                         | OP                   | NA                            |                                          |                                         |
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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.104937.

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