

Variant/Phase Distribution Model for FePd

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Introduction

Ferromagnetic shape memory alloys (FSMAs) have received attention recently because of their ability to produce large strains in the presence of an external magnetic field. These strains can be an order of magnitude larger than those produced by alloys with a strong magnetostrictive coupling. Terfenol-D has produced strains as large as 0.24% while the FSMA Ni-Mn-Ga has demonstrated strains of 6%.[1] This order of magnitude difference in strain results from the operation of dissimilar mechanisms, the first is produced by typical magnetostriction and the second results from the reorientation of martensite twins.

FSMAs that produce large field induced strains have a twinned martensite structure with high magnetocrystalline anisotropy. When subjected to a magnetic field, the Zeeman energy causes a material to align its magnetic moment in the direction of the field. The magnetocrystalline anisotropy wants to align the field in a certain crystallographic direction. In FSMAs the path with the lowest energy barrier to equilibrate these driving forces is twin boundary motion. The boundary moves into the unfavorably oriented twin and away from the favorably oriented twin (Figure 1).

Image removed due to copyright considerations. See reference [2].

As the twin boundary moves the shape anisotropy of the crystal lattice causes deformation of the material. The axis of easy magnetization lies along a particular direction(s) in the martensite. This direction corresponds to a different lattice parameter than the hard magnetization direction(s). So as the twin boundary moves to align the magnetic moment with the field it is also aligning the lattice parameter that corresponds to the easy direction. This strains the material by the difference in the lattice parameters.

Another possible mechanism for producing large strains in FSMAs is the field-induced austenite to martensite phase transformation. This phase transition is another typical characteristic of FSMAs, although it is usually activated thermally or mechanically. The high crystal symmetry austenite phase has a different lattice parameter than the martensite phase. So phase boundary motion will also strain the material (Figure 2). This paper presents a simple phenomenological model that demonstrates magnetic field induced twin boundary motion and austenite-martensite phase transformation, resulting in large recoverable strains.

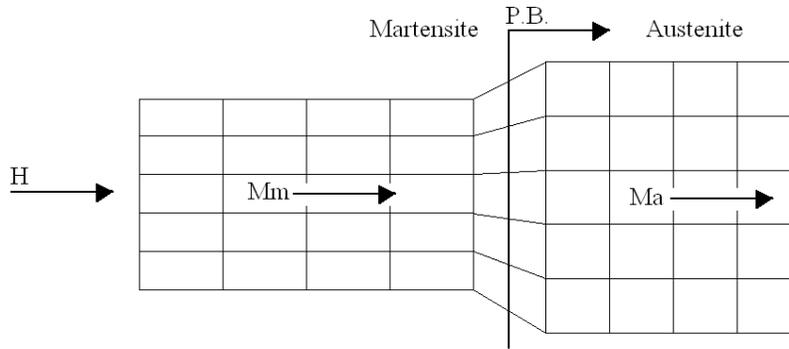


Figure 2: Field induced phase boundary motion

This paper investigates the specific case: unconstrained deformation of single crystal multiphase iron palladium (FePd) when subjected to a magnetic field. First a description of the austenite and martensite phases is presented, then an overview of the governing energetics and finally an analytical quantitative analysis of the strain as a function of external magnetic field.

Austenite and Martensite Phase In FePd

FePd is a promising FSMA for device applications. FePd has high magnetocrystalline anisotropy, which facilitates twin boundary motion. Also FePd is ductile in both phases. This improves reliability for actuator type devices over brittle Ni-Mn-Ga.

The root cause of the shape memory effect (SME) in FePd is an austenite to martensite solid state phase transformation. In the austenite phase FePd has a face centered cubic (FCC) crystal structure and in the martensite phase, a face centered tetragonal structure (FCT) (Figure 3).

Image removed due to copyright considerations. See reference [5].

Referring to figure 3, it can be seen that the martensite phase is elongated on two sides and shortened on one side when compared to the austenite phase. This microscopic change of shape causes macroscopic deformations as the entire sample switches phase. It is also important to note the easy axes of magnetization. The martensite phase of FePd demonstrates high magnetic anisotropy, favoring to magnetize in the elongated directions, indicated with arrows $[a\ 0\ 0]$. Conversely austenite has low magnetic anisotropy with hard directions along $[a\ 0\ 0]$, again indicated with arrows.

The martensite phase creates internal stresses as it nucleates and grows within the austenite phase. The stresses become large enough to necessitate compensation. This can be accomplished by twinning or slip (Figure 4).

Image removed due to copyright considerations. See reference [2].

Both methods of compensation have energy barriers and equilibrium conditions. The energy barrier to twin is smaller than the energy required to slip. This can be shown analytically and is experimentally observable.[3,4] Fortunately FePd prefers to twin rather than slip because it is precisely this that allows for large strains in the martensite phase.

FePd can also produce large strains through an austenite-martensite phase transformation. Here it is phase boundary motion that consumes the unfavorable phase. The energetics of this transformation are detailed in the following sections.

Governing Energetics

When considering the preferred state of a system, energy equilibrium is the place to start. The current system has 3 main types of governing energy; magnetic, mechanical, and latent heat. Each type of energy is now discussed in detail.

Magnetic Energy

The possible contributors to magnetic energy in a system of this type are; exchange, domain wall, magnetostatic, magnetoelastic, magnetocrystalline anisotropy and Zeeman energy. As alluded to previously, the most important energies of this specific system are magnetocrystalline anisotropy and Zeeman. What follows is justification for this assumption and quantitative representations of these energies.

Exchange energy represents the energy cost of adjacent magnetic moments pointing in different directions. For this model it is assumed that the martensite twins and austenite are single domain, therefore there will be no exchange energy contribution from within each variant/phase. However domains do exist between twins and between phases. It has been shown that the exchange energy is significant when compared to other energies of this system. In fact the exchange energy is large enough so that creating a single variant/single phase sample is rarely possible. So this energy will be a constant in the system. For this reason the *change* in energy of twin/phase boundary motion will not be a function of the exchange energy and can be omitted.[2]

Domain wall energy is a combination of exchange energy and magnetocrystalline anisotropy or magnetostatic energy. The domain wall reduces the magnetocrystalline energy by rotating the magnetic moment gradually over the thickness of the wall. This comes at a cost of orienting the magnetic moment in an energetically undesirable crystallographic orientation or by creating free poles at wall boundaries. The energy contribution from domain walls can be neglected for the same reason as neglecting exchange energy given above.

Magnetostatic energy arises from poles at an interface. Here it is assumed that the normal component of magnetization is continuous across the twin/phase boundary interface. This has been proved for the twin boundary case.[4] Therefore magnetostatic energy contribution is nil.

Magnetocrystalline anisotropy arises from the magnetization in a material having a preferred crystallographic direction. As the magnetization moves away from this direction, by an off axis field, the material becomes harder to magnetize. So for a given magnetization the energy is lowest in the easy direction and highest in the hard direction. The magnetocrystalline anisotropy energy per unit volume is quantified to leading order as

$$(1) \quad u_a = K_u \sin^2[\theta] \dots \text{uniaxial}$$

$$(2) \quad u_a = K_1 (\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_1^2 \alpha_3^2) \dots \text{cubic}$$

Magnetoelastic energy is magnetocrystalline anisotropy that is proportional to the strain of the lattice. Because the strain from twin/phase boundary motion is much larger than the lattice strain this energy can be neglected.

The Zeeman energy is the potential energy of a magnetic moment in a magnetic field. This is the energy that tends to align the magnetic moment with the applied field. Written as energy per unit volume, the Zeeman energy is quantified as

$$(3) \quad u_z = -\mathbf{M}_s \cdot \mathbf{H}$$

Mechanical Energy

The mechanical energy associated with this system is the well know continuum mechanics strain energy. This energy opposes the motion of twin/phase boundaries. It is quantified as

$$(4) \quad U_e = \frac{1}{2} C_{\text{eff}} e_{ij}^2$$

Latent Heat

Latent heat is the energy associated with the phase change in a material. The austenite to martensite transformation is exothermic. The energy per unit volume is simply

$$(5) \quad u_L = 10.79 \left(\frac{\text{erg}}{\text{cm}^3} \right) \quad [5]$$

Analysis

For the purposes of this paper further assumptions can be made to simplify the energetics. First a 2D simulation reduces the number of variants for the analytical analysis. The analysis presented is, in general, valid in full 3D form however it is cumbersome to deal with all variants in the analytical calculations. This assumptions lead to the following arrangement (Figure 5).

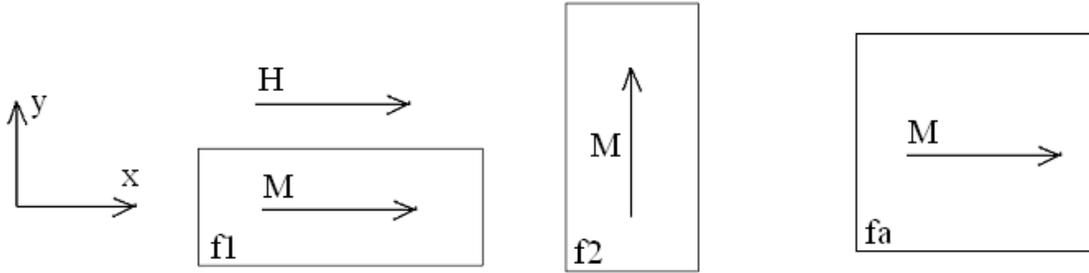


Figure 5: 2D FePd martensite variants (f_1, f_2) and austenite phase (f_a)

To further simplify the calculation the applied field (H) is along the direction of easy magnetization of variant 1, and the twinning angle between variants is 90° . Here f_1, f_2 and f_a are the respective volume fractions. With these simplifications the total Zeeman energy for the system becomes

$$(6) \quad U_z = -M_{sa} H f_a - M_{sm} \cdot H f_1$$

Here the subscripts “a” and “m” refer to austenite and martensite respectively. It is assumed that the anisotropy of the martensite phase is strong enough to keep the magnetic moment of variant 2 orthogonal to the field, therefore it does not contribute to the Zeeman energy.

The simplifications lead to a magnetocrystalline anisotropy energy of

$$(7) \quad U_a = K_u \left(\frac{M_{sm} H}{2 K_u} \right)^2 f_2 + K_1 \left(\frac{M_{sa} H}{2 K_1} \right)^2 f_a$$

Here the cosine of the angle between the field and magnetization is written as a ratio of the Zeeman and magnetocrystalline anisotropy energies. Martensite variant 1 is magnetized along its easy direction and therefore does not contribute to the anisotropy energy.

With the reduced dimensions, a good approximation to the strain energy is

$$(8) \quad U_e = \frac{1}{2} C_{eff} (e_x^2 + e_y^2)$$

where,

$$e_x = \frac{((f_1 a + f_2 c + f_a a_0) - (f_{10} a + f_{20} c + f_{a0} a_0))}{(f_{10} a + f_{20} c + f_{a0} a_0)}$$

$$e_y = \frac{((f_1 c + f_2 a + f_a a_0) - (f_{10} c + f_{20} a + f_{a0} a_0))}{(f_{10} a + f_{20} c + f_{a0} a_0)}$$

Here “Ceff” is the effective material modulus ($C_{eff} = 100 \cdot 10^9$ Pa), “fxo” denotes an initial volume fraction ($f_{x0} = 1/3$), “c” is the shortened martensite lattice parameter ($c = 3.630 \cdot 10^{-10}$ m), “a” is the elongated lattice parameter ($a = 3.822 \cdot 10^{-10}$ m), and “ao” is the austenite lattice parameter ($a_0 = 3.756 \cdot 10^{-10}$ m).[5]

The final energy contribution, the latent heat, is written as

$$(9) \quad U_L = u_L (f_a - f_{a0})$$

Combining equations 6-9 gives the total energy of the system.

$$(10) \quad U = -M_{sa} H f_a - M_{sm} H f_1 + K_u \left(\frac{M_{sm} H}{2 K_u} \right)^2 f_2 + K_1 \left(\frac{M_{sa} H}{2 K_1} \right)^2 f_a + \frac{1}{2} C_{eff} (e_x^2 + e_y^2) + u_L (f_a - f_{a0})$$

The minimum of equation 10 subject to the constraint

$$(11) \quad f_1 + f_2 + f_a = 1$$

gives the variant/phase distribution of the material as a function of the applied field. Once this is known, useful information like average magnetization and strain is easily extracted. This problem is solved using the Lagrangian multiplier method. The full solution is given in Appendix A, results are given in the following section.

Applying the Lagrangian multiplier method to equations 10 & 11 results in three equations of 5 variables

$$(12)$$

$$\begin{aligned}
& -1.99465 \times 10^{12} + 1.99063 \times 10^{12} f_1 + 1.98799 \times 10^{12} f_2 + 2.00532 \times 10^{12} f_a - 1220 \cdot H = 2 f_1 \lambda_m, \\
& -1.99465 \times 10^{12} + 1.98799 \times 10^{12} f_1 + 1.99063 \times 10^{12} f_2 + 2.00532 \times 10^{12} f_a + 1.0912 H^2 = 2 f_2 \lambda_m, \\
& -2.0106 \times 10^{12} + 2.00532 \times 10^{12} f_1 + 2.00532 \times 10^{12} f_2 + 2.02147 \times 10^{12} f_a - 1080 \cdot H - 58.32 H^2 = 2 f_a \lambda_m
\end{aligned}$$

A plausible value for lambda can be found by remembering the initial condition ($H_0 = 0$, $f_{10} = f_{20} = f_{a0} = 1/3$). Then with the value of lambda known, the volume fractions can be solved for as a function of the field.

Results

For low magnetic fields ($H \sim 1$ kOe) the volume fraction distribution is shown in figure 6.

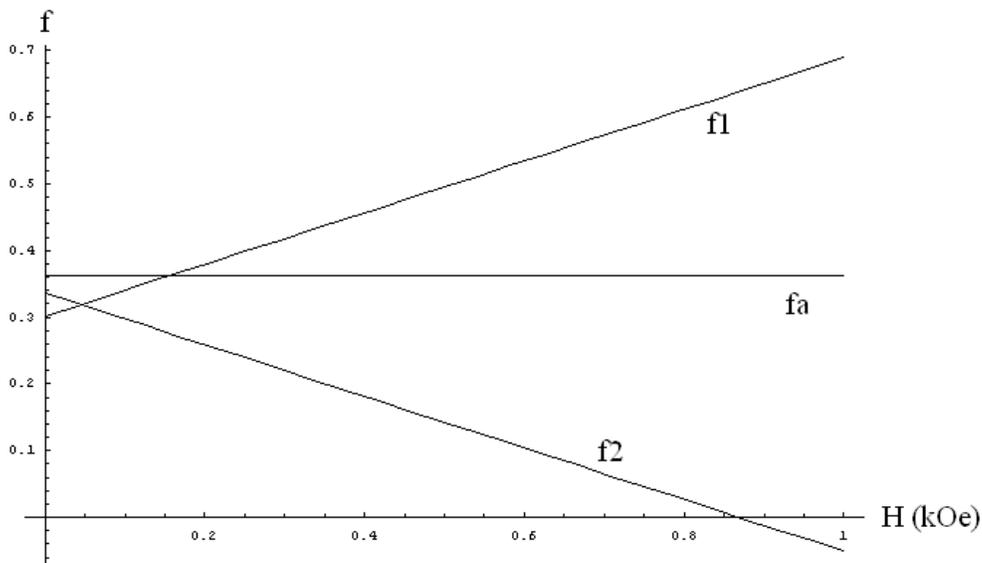


Figure 6: Martensite variant and austenite volume fraction in the low field regime

This figure shows that low magnetic fields have a large effect on the martensite variant distribution and little effect on the phase distribution. The f_2 variant is completely consumed (This is a good approximation with the qualification that exchange energy prohibits complete consumption) by the f_1 variant, while the f_a fraction remains essentially constant. It is obvious that the volume fraction of f_2 cannot be negative therefore a second high field solution was generated where the initial volume fractions are $f_{10} = 2/3$ and $f_{a0} = 1/3$. The solution to this high field situation is given in appendix B. The high magnetic field ($H \sim 1000$ kOe) volume fraction distribution is shown in figure 7.

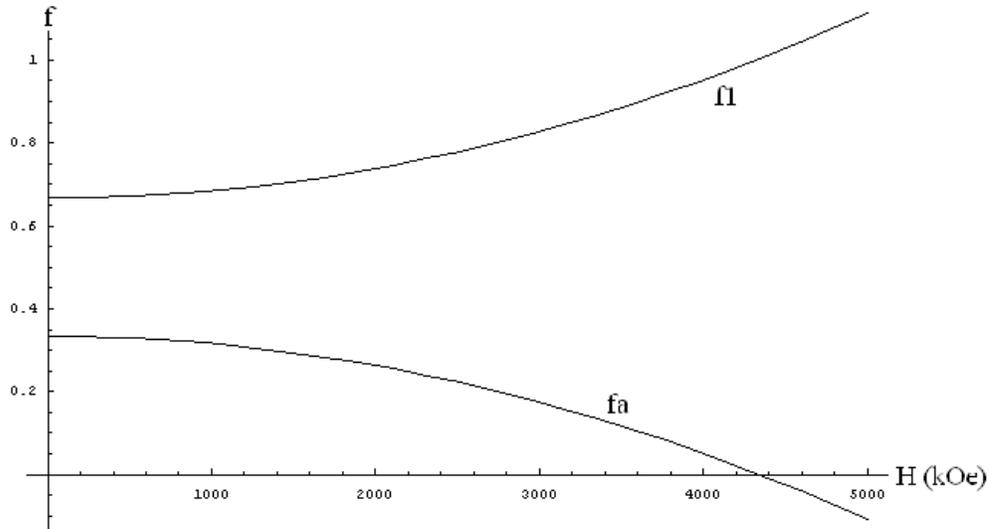


Figure 7: Martensite variant and austenite volume fraction in the high field regime

This figure shows that a high magnetic field can produce a phase transformation. The austenite phase is completely consumed (This is a good approximation with the qualification that exchange energy prohibits complete consumption) by the single variant martensite phase.

With the variant fractions known, the strain can be calculated using the definition provided for equation 8. The low field strain is shown in figure 8.

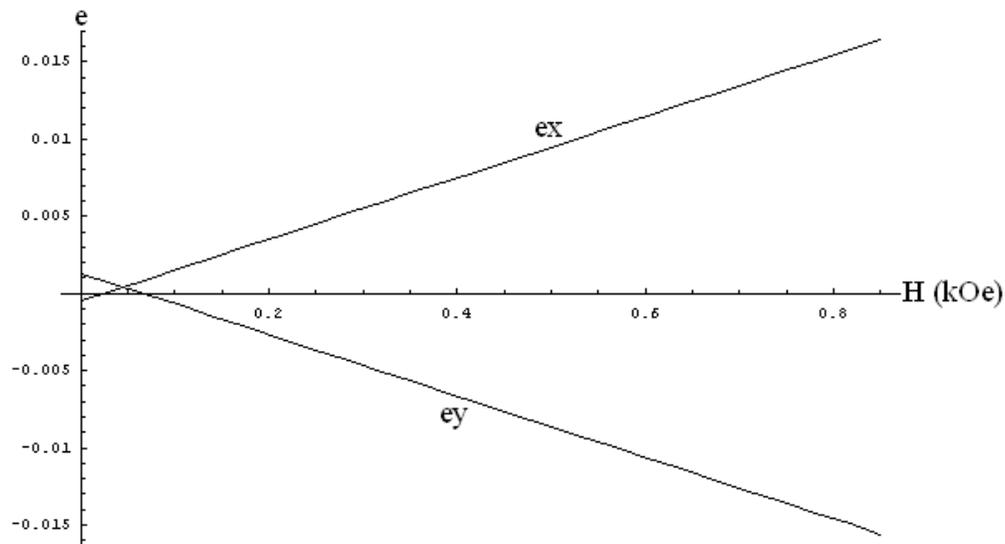


Figure 8: Strain in the low magnetic field regime

This figure shows the expected positive strain in the direction of applied field and negative strain in the orthogonal direction. Also it can be seen that the strain is nearly linear with the applied field in the low field regime. The high field strain is shown in figure 9.

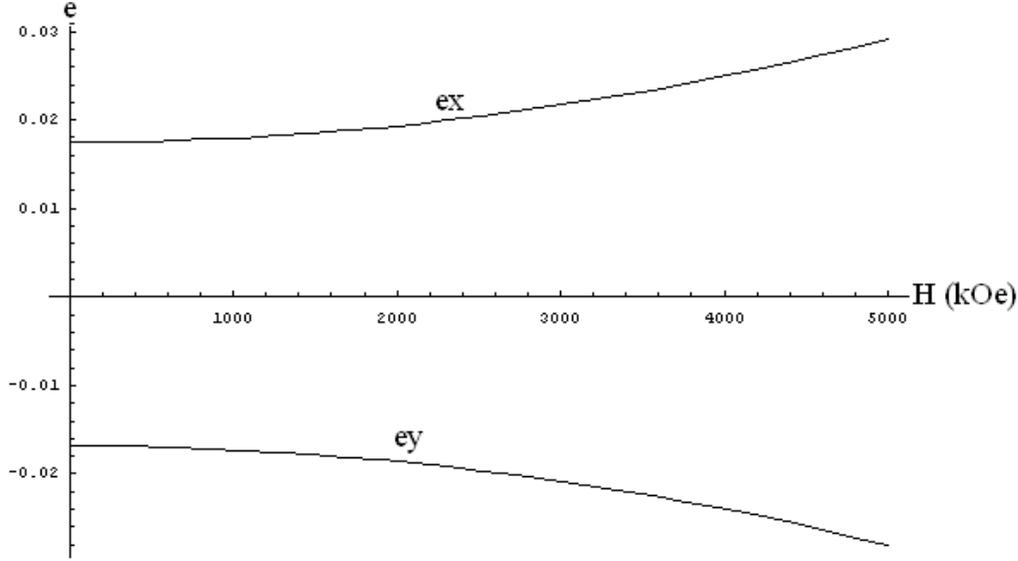


Figure 9: Strain in the high magnetic field regime

This figure shows a continued positive strain in the field direction and contraction orthogonal to the field. In the high field regime the material has a nonlinear strain response to the applied field. The total strain for the given initial conditions is $\sim 3\%$.

Discussion

As seen in figures 8 and 9, FePd has 2 distinct strain response regimes for an applied magnetic field. This is the result of 2 different mechanisms. In the low field regime the strain is a result of twin boundary motion and in the high field regime the strain is a result of phase boundary motion. This is determined from the fact that the austenite volume fraction remain approximately unchanged in the low field regime and in the high field regime there is only one variant of martensite so the only mechanism to create strain is phase boundary motion. With this consideration, the f_a terms can be removed from equation 10 to simplify the energetics of the low field regime. This modification clarifies the energetics to

$$(13) \quad U = -f_1 M_{sm} H + \frac{f_2 H^2 M_{sm}^2}{4 K_u} + \frac{1}{2} C_{eff} (e_x^2 + e_y^2)$$

The Zeeman energy of the f_1 variant and the magnetocrystalline anisotropy energy of the f_2 variant drive the twin boundary while the elastic energy opposes the motion. Similarly, removing the f_2 terms from equation 10 clarifies the energetics of the high field regime.

$$(14) \quad U = -f_1 H M_{sm} + \frac{f_a H^2 M_{sa}^2}{4 K_l} + (f_a - f_{a0}) u_L - f_a H M_{sa} + \frac{1}{2} C_{eff} (e_x^2 + e_y^2)$$

The Zeeman energy of the f1 variant, and magnetocrystalline anisotropy energy and the latent heat of fa drive the phase boundary while the Zeeman energy of fa and elastic energy oppose the motion. Equations 13 and 14 quantify the energetics of the two mechanisms that drive the magnetically induced strain in FePd.

Conclusion

A simple model has been presented to describe the field induced strain in FSMA FePd. The model demonstrates two regimes of strain response. The active mechanism in the low field regime is twin boundary motion while the mechanism in the high field regime is phase boundary motion.

For evenly dispersed initial volume fractions the material strained ~3% while approximately fully transforming into the favorably oriented martensite variant. The amount of strain induced in the low and high magnetic field regimes is ~1.5%. The low field regime is 3 orders of magnitude more efficient at producing strain when compared to the high field regime (by comparing the applied fields). However the high field response is still valuable because it can be used to fully transform the material into the martensite phase, which is not always possible using typical metallurgical techniques. Also this allows the material to realize its full strain capabilities.

References

- [1] S.J. Murray, M. Marioni, S.M. Allen, R.C. O'Handley, *App. Phys. Let.*, Vol. 77, No.6, 2000
- [2] R. C. O'Handley, *J. of App. Phys.*, Vol. 83, No. 6, 1998.
- [3] H. Kato et. al., *Mat. Sci. & Eng.*, A322, 2002
- [4] R. D. James and M. Wuttig, *Phil. Mag. A*, Vol. 77, No. 5, 1998.
- [5] J. Cui, T.W. Shield, R.D. James, *Acta Materialia*, Vol. 52, 2004
- [6] R.C. O'Handley, *Modern Magnetic Materials*, Wiley-Interscience, 1999

Appendix A

Volume Distribution Solution - Low Magnetic Field

■ Programming Options

```
Needs["OptimizationToolbox`QuadraticProgramming`"];
Off[General::"spell1"]
Off[General::"spell"]
<< Calculus`VectorAnalysis`
```

■ Energies

Zeeman energy

```
Uz1 = - (f1) Msm H ;
Uz2 = 0 ;
Uza = - (fa) Msa H ;
Uz = Uz1 + Uz2 + Uza ;
```

Anisotropy energy

```
Ua1 = 0 ;
Ua2 = (f2) Ku (Msm H / 2 / Ku) ^ 2 ;
Uaa = (fa) K1 (Msa H / 2 / K1) ^ 2 ;
Ua = Ua1 + Ua2 + Uaa ;
```

Strain energy relative to initial condition

```
ex = ((f1 a + f2 c + fa ao) - (f1o a + f2o c + fao ao)) / (f1o a + f2o c + fao ao) ;
ey = ((f1 c + f2 a + fa ao) - (f1o c + f2o a + fao ao)) / (f1o c + f2o a + fao ao) ;
Ue = 10 * Ceff (ex^2 + ey^2) / 2 ;
```

Latent Heat

```
U1 = (fa - fao) L ;
```

Total energy

U = Simplify[Uz + Ua + Ue + U1]

5 Ceff

$$\left(\frac{(c(f1 - f1o) + a(f2 - f2o) + ao(fa - fao))^2}{(c f1o + a f2o + ao fao)^2} + \frac{(a(f1 - f1o) + c(f2 - f2o) + ao(fa - fao))^2}{(a f1o + c f2o + ao fao)^2} \right) + (fa - fao) L - fa H Msa + \frac{fa H^2 Msa^2}{4 K1} - f1 H Msm + \frac{f2 H^2 Msm^2}{4 Ku}$$

■ Langrangian Multiplier Method

Equating the gradient of the extreme value function to the gradient of the constraining function multiplied by lambda

Gradient of the energy equation with respect to the variant fractions

GradU = Grad[U, Cartesian[f1, f2, fa]]

$$\left\{ \begin{aligned} &5 \text{ Ceff} \left(\frac{2 c (c (f1 - f1o) + a (f2 - f2o) + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 a (a (f1 - f1o) + c (f2 - f2o) + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) - H Msm, \\ &5 \text{ Ceff} \left(\frac{2 a (c (f1 - f1o) + a (f2 - f2o) + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 c (a (f1 - f1o) + c (f2 - f2o) + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) + \frac{H^2 Msm^2}{4 Ku}, \\ &5 \text{ Ceff} \left(\frac{2 ao (c (f1 - f1o) + a (f2 - f2o) + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 ao (a (f1 - f1o) + c (f2 - f2o) + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) + L - H Msa + \frac{H^2 Msa^2}{4 K1} \end{aligned} \right\}$$

Gradient of the constraint equation

GradF = Grad[lam * (f1² + f2² + fa² - 1), Cartesian[f1, f2, fa]]

{2 f1 lam, 2 f2 lam, 2 fa lam}

Equating the gradient of the extreme value function to the gradient of the constraining function

eqns = {GradU[[1]] == GradF[[1]], GradU[[2]] == GradF[[2]], GradU[[3]] == GradF[[3]]}

$$\left\{ \begin{aligned} &5 \text{ Ceff} \left(\frac{2 c (c (f1 - f1o) + a (f2 - f2o) + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 a (a (f1 - f1o) + c (f2 - f2o) + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) - H Msm == 2 f1 lam, \\ &5 \text{ Ceff} \left(\frac{2 a (c (f1 - f1o) + a (f2 - f2o) + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 c (a (f1 - f1o) + c (f2 - f2o) + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) + \frac{H^2 Msm^2}{4 Ku} == 2 f2 lam, \\ &5 \text{ Ceff} \left(\frac{2 ao (c (f1 - f1o) + a (f2 - f2o) + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 ao (a (f1 - f1o) + c (f2 - f2o) + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) + L - H Msa + \frac{H^2 Msa^2}{4 K1} == 2 fa lam \end{aligned} \right\}$$

■ Numerical Parameters [5]

Lattice parameters

$$\begin{aligned} a_0 &= 3.756 \times 10^{-10} \text{ (nm)}; \\ a &= 3.822 \times 10^{-10} \text{ (nm)}; \\ c &= 3.630 \times 10^{-10} \text{ (nm)}; \end{aligned}$$

Saturation magnetization relative to each variant

$$\begin{aligned} M_{sm} &= 1220 \text{ (emu/cm}^3\text{)}; \\ M_{sa} &= 1080 \text{ (emu/cm}^3\text{)}; \end{aligned}$$

Anisotropy constants

$$\begin{aligned} K_u &= 3.41 \times 10^5 \text{ (erg/cm}^3\text{)}; \\ K_1 &= -5 \times 10^3 \text{ (erg/cm}^3\text{)}; \end{aligned}$$

Effective modulus

$$C_{eff} = 100 \times 10^9 \text{ (Pa)};$$

Latent heat fcc-fct

$$L = 10.79 \times 10^7 \text{ (erg/cm}^3\text{)};$$

Initial volume fraction

$$\begin{aligned} f_{1o} &= 1/3; \\ f_{2o} &= 1/3; \\ f_{ao} &= 1/3; \end{aligned}$$

■ Solving for Volume Fraction

`simpeqns[H_] = Simplify[eqns]`

$$\begin{aligned} \{-1.99465 \times 10^{12} + 1.99063 \times 10^{12} f_1 + 1.98799 \times 10^{12} f_2 + 2.00532 \times 10^{12} f_a - 1220. H == 2 f_1 \lambda_m, \\ -1.99465 \times 10^{12} + 1.98799 \times 10^{12} f_1 + 1.99063 \times 10^{12} f_2 + 2.00532 \times 10^{12} f_a + 1.0912 H^2 == 2 f_2 \lambda_m, \\ -2.0106 \times 10^{12} + 2.00532 \times 10^{12} f_1 + 2.00532 \times 10^{12} f_2 + \\ 2.02147 \times 10^{12} f_a - 1080. H - 58.32 H^2 == 2 f_a \lambda_m\} \end{aligned}$$

Solving for the variant fractions that minimize the energy as a function of applied field

```

fsol = Solve[simpeqns[H], {f1, f2, fa}];
f1[H_, lam_] = f1 /. fsol[[1, 1]]
f2[H_, lam_] = f2 /. fsol[[1, 2]]
fa[H_, lam_] = fa /. fsol[[1, 3]]

-4.98672×10-13 (-2.0106×1012 - 1080. H - 58.32 H2) +
(4.98672×10-13 (-1. (-1.98799×1012 (-2.0106×1012 - 1080. H - 58.32 H2) +
2.00532×1012 (-1.99465×1012 + 1.0912 H2))
(3.98656×1024 - 2.00532×1012 (1.99063×1012 - 2. lam)) +
(2.00532×1012 (-1.99465×1012 - 1220. H) - 1. (-2.0106×1012 - 1080. H - 58.32 H2)
(1.99063×1012 - 2. lam)) (5.29631×1021 - 4.01065×1012 lam))
(2.02147×1012 - 2. lam) / (-5.6871×1030 + 6.35566×1034 lam -
4.81497×1025 lam2 + 1.60426×1013 lam3) +
1. ((-1.98799×1012 (-2.0106×1012 - 1080. H - 58.32 H2) +
2.00532×1012 (-1.99465×1012 + 1.0912 H2)) / (5.29631×1021 - 4.01065×1012 lam) -
(1. (-1. (-1.98799×1012 (-2.0106×1012 - 1080. H - 58.32 H2) +
2.00532×1012 (-1.99465×1012 + 1.0912 H2))
(3.98656×1024 - 2.00532×1012 (1.99063×1012 - 2. lam)) +
(2.00532×1012 (-1.99465×1012 - 1220. H) - 1. (-2.0106×1012 - 1080. H - 58.32 H2)
(1.99063×1012 - 2. lam)) (5.29631×1021 - 4.01065×1012 lam))
(4.02133×1024 - 1.98799×1012 (2.02147×1012 - 2. lam))) /
((5.29631×1021 - 4.01065×1012 lam)
(-5.6871×1030 + 6.35566×1034 lam - 4.81497×1025 lam2 + 1.60426×1013 lam3)))

-(1. (-1.98799×1012 (-2.0106×1012 - 1080. H - 58.32 H2) +
2.00532×1012 (-1.99465×1012 + 1.0912 H2)) / (5.29631×1021 - 4.01065×1012 lam) +
((-1. (-1.98799×1012 (-2.0106×1012 - 1080. H - 58.32 H2) + 2.00532×1012 (-1.99465×1012 +
1.0912 H2)) (3.98656×1024 - 2.00532×1012 (1.99063×1012 - 2. lam)) +
(2.00532×1012 (-1.99465×1012 - 1220. H) - 1. (-2.0106×1012 - 1080. H - 58.32 H2)
(1.99063×1012 - 2. lam)) (5.29631×1021 - 4.01065×1012 lam))
(4.02133×1024 - 1.98799×1012 (2.02147×1012 - 2. lam))) /
((5.29631×1021 - 4.01065×1012 lam)
(-5.6871×1030 + 6.35566×1034 lam - 4.81497×1025 lam2 + 1.60426×1013 lam3)))

-(1. (-1. (-1.98799×1012 (-2.0106×1012 - 1080. H - 58.32 H2) +
2.00532×1012 (-1.99465×1012 + 1.0912 H2))
(3.98656×1024 - 2.00532×1012 (1.99063×1012 - 2. lam)) +
(2.00532×1012 (-1.99465×1012 - 1220. H) - 1. (-2.0106×1012 - 1080. H - 58.32 H2)
(1.99063×1012 - 2. lam)) (5.29631×1021 - 4.01065×1012 lam))) /
(-5.6871×1030 + 6.35566×1034 lam - 4.81497×1025 lam2 + 1.60426×1013 lam3))

```

Solving for lambda

```

sol1 = Solve[f1[0, lam] == 1 / 3, lam]
sol2 = Solve[f2[0, lam] == 1 / 3, lam]
sola = Solve[fa[0, lam] == 1 / 3, lam]
lambda = lam /. sol1[[2]]

{{lam -> -9.32668 × 109}, {lam -> 1.32056 × 109}, {lam -> 1.32056 × 109}, {lam -> 1.73996 × 1010}}

{{lam -> -9.32668 × 109}, {lam -> 1.32056 × 109 - 789.133 i},
 {lam -> 1.32056 × 109 + 789.133 i}, {lam -> 1.73996 × 1010}}

{{lam -> -7.92756 × 109 - 1.60973 × 1010 i}, {lam -> -7.92756 × 109 + 1.60973 × 1010 i}}

1.32056 × 109

```

Checking the initial volume fraction distribution

```

f1[0, lambda]
f2[0, lambda]
fa[0, lambda]

0.301865

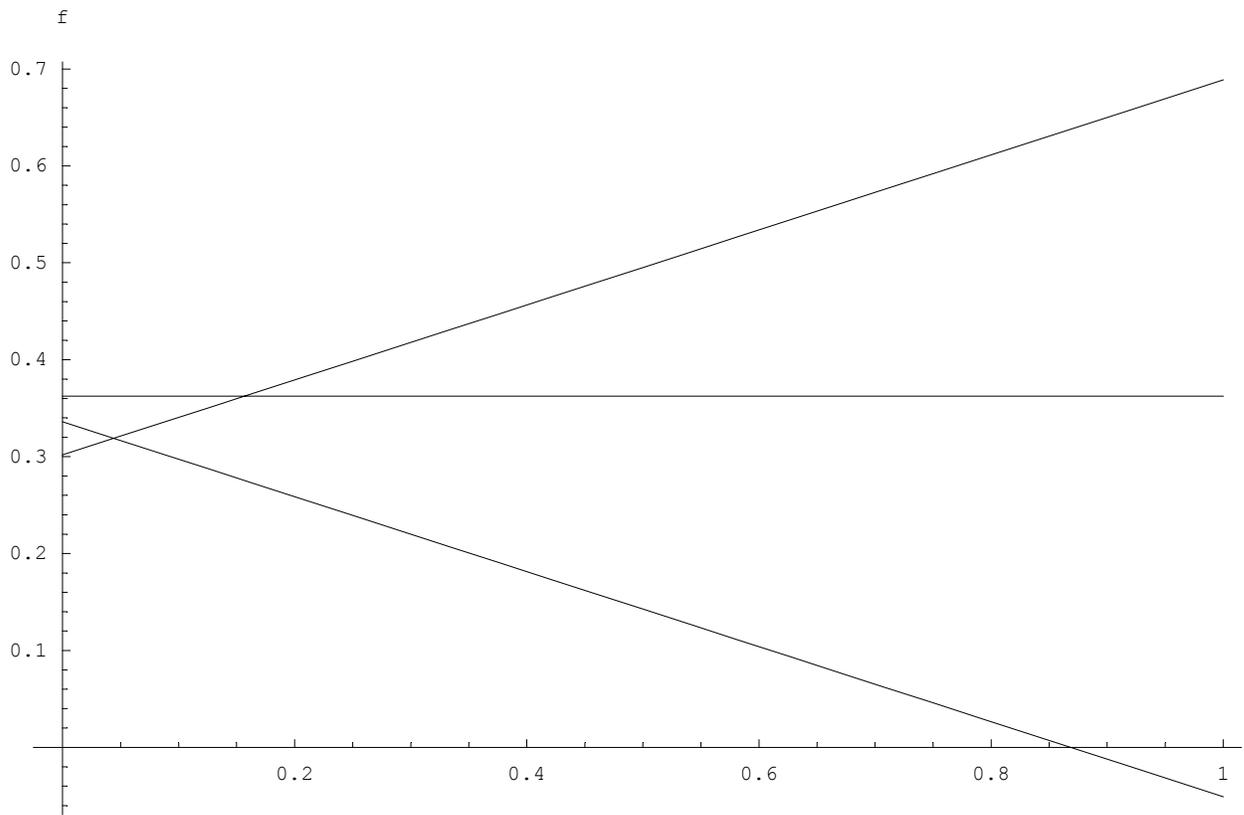
0.335981

0.362344

```

Volume fraction distribution vs. applied field

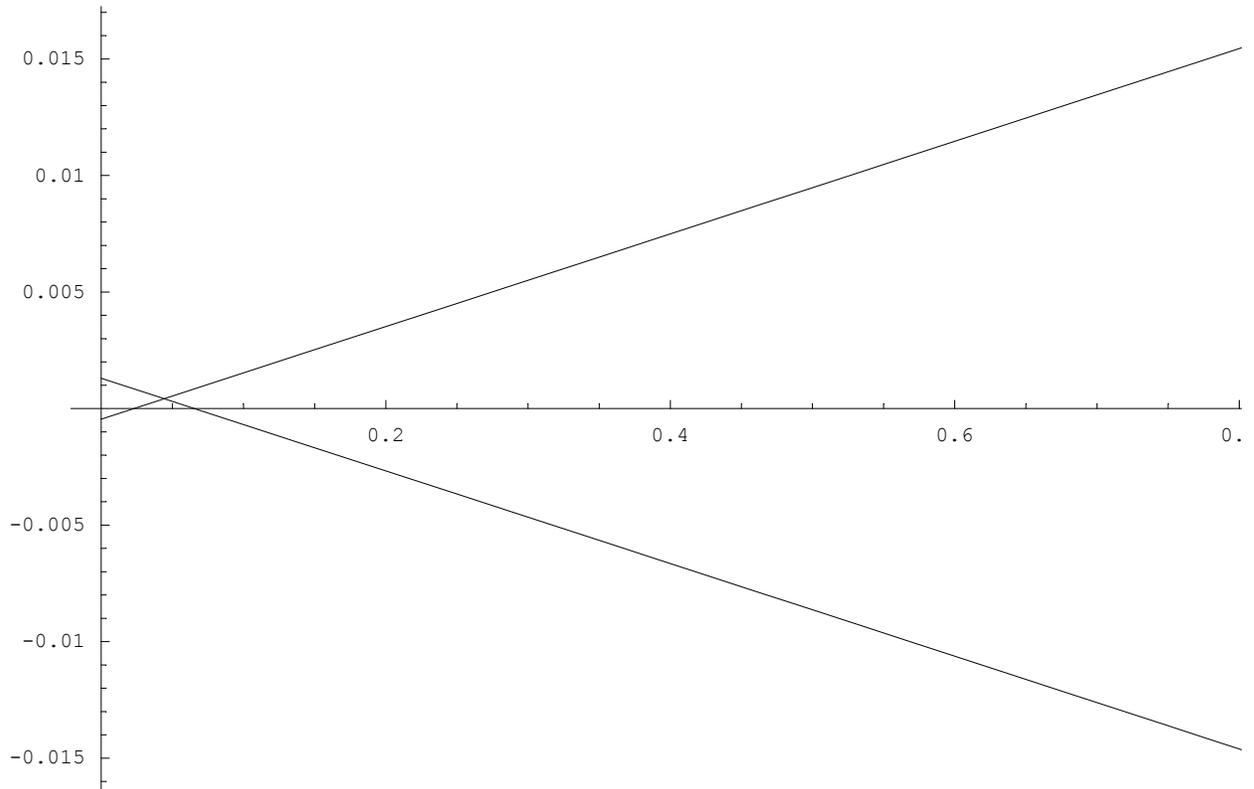
```
Plot[{f1[H, lambda], f2[H, lambda], fa[H, lambda]},  
      {H, 0, 1}, AxesOrigin -> {0, 0}, AxesLabel -> {"H (kOe)", "f"}]
```



- Graphics -

Strain vs. applied field

```
exh[H_] = ((f1[H, lambda] a + f2[H, lambda] c + fa[H, lambda] ao) - (f1o a + f2o c + fao ao)) /  
  (f1o a + f2o c + fao ao);  
eyh[H_] = ((f1[H, lambda] c + f2[H, lambda] a + fa[H, lambda] ao) - (f1o c + f2o a + fao ao)) /  
  (f1o c + f2o a + fao ao);  
Plot[{exh[H], eyh[H]}, {H, 0, .85}]
```



- Graphics -

Appendix B

Volume Distribution Solution - High Magnetic Field

■ Programming Options

```
Needs["OptimizationToolbox`QuadraticProgramming`"];
Off[General::"spell1"]
Off[General::"spell"]
<< Calculus`VectorAnalysis`
```

■ Energies

Zeeman energy

```
Uz1 = - (f1) Msm H ;
Uz2 = 0 ;
Uza = - (fa) Msa H ;
Uz = Uz1 + Uz2 + Uza ;
```

Anisotropy energy

```
Ua1 = 0 ;
Ua2 = 0 ;
Uaa = (fa) K1 (Msa H / 2 / K1) ^ 2 ;
Ua = Ua1 + Ua2 + Uaa ;
```

Strain energy relative to initial condition

```
ex = ((f1 a + fa ao) - (f1o a + f2o c + fao ao)) / (f1o a + f2o c + fao ao) ;
ey = ((f1 c + fa ao) - (f1o c + f2o a + fao ao)) / (f1o c + f2o a + fao ao) ;
Ue = 10 * Ceff (ex^2 + ey^2) / 2 ;
```

Latent Heat

```
U1 = (fa - fao) L ;
```

Total energy

U = Simplify[Uz + Ua + Ue + U1]

$$5 \text{ Ceff} \left(\frac{(c (f1 - f1o) - a f2o + ao (fa - fao))^2}{(c f1o + a f2o + ao fao)^2} + \frac{(a (f1 - f1o) - c f2o + ao (fa - fao))^2}{(a f1o + c f2o + ao fao)^2} \right) +$$

$$(fa - fao) L - fa H Msa + \frac{fa H^2 Msa^2}{4 K1} - f1 H Msm$$

■ Langrangian Multiplier Method

Here the equation to be minimized is the energy equation and the constraining equation is the volume fractions

Gradient of the energy equation with respect to the variant fractions

GradU = Grad[U, Cartesian[f1, fa, z]]

$$\left\{ 5 \text{ Ceff} \left(\frac{2 c (c (f1 - f1o) - a f2o + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 a (a (f1 - f1o) - c f2o + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) - \right.$$

$$\left. H Msm, \right.$$

$$5 \text{ Ceff} \left(\frac{2 ao (c (f1 - f1o) - a f2o + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 ao (a (f1 - f1o) - c f2o + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) +$$

$$\left. L - H Msa + \frac{H^2 Msa^2}{4 K1}, 0 \right\}$$

Gradient of the constraint equation

GradF = Grad[lam * (f1² + fa² - 1), Cartesian[f1, fa, z]]

$$\{2 f1 \text{ lam}, 2 fa \text{ lam}, 0\}$$

Equating the gradient of the extreme value function to the gradient of the constraining function multiplied by lambda

eqns = {GradU[[1]] == GradF[[1]], GradU[[2]] == GradF[[2]]}

$$\left\{ 5 \text{ Ceff} \left(\frac{2 c (c (f1 - f1o) - a f2o + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 a (a (f1 - f1o) - c f2o + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) - \right.$$

$$\left. H Msm == 2 f1 \text{ lam}, \right.$$

$$5 \text{ Ceff} \left(\frac{2 ao (c (f1 - f1o) - a f2o + ao (fa - fao))}{(c f1o + a f2o + ao fao)^2} + \frac{2 ao (a (f1 - f1o) - c f2o + ao (fa - fao))}{(a f1o + c f2o + ao fao)^2} \right) +$$

$$\left. L - H Msa + \frac{H^2 Msa^2}{4 K1} == 2 fa \text{ lam} \right\}$$

■ Numerical Parameters [5]

Lattice parameters

$$ao = 3.756 * 10^{-10} \text{ (*m*)};$$

$$a = 3.822 * 10^{-10} \text{ (*m*)};$$

$$c = 3.630 * 10^{-10} \text{ (*m*)};$$

Saturation magnetization relative to each variant

```
Msm = 1220 (*emu/cm3*) ;
Msa = 1080 (*emu/cm3*) ;
```

Anisotropy constants

```
Ku = 3.41 * 105 (*erg/cm3*) ;
K1 = -5 * 103 (*erg/cm3*) ;
```

Effective modulus

```
Ceff = 100 * 109 (*Pa*) ;
```

Latent heat fcc-fct

```
L = 10.79 * 107 (*erg/cm3*) ;
```

Initial volume fraction

```
f1o = 1 / 3 ;
f2o = 1 / 3 ;
fao = 1 / 3 ;
```

■ Solving for Volume Fraction

```
simpeqns[H_] = Simplify[eqns]
{-1.99465 × 1012 + 1.99063 × 1012 f1 + 2.00532 × 1012 fa - 1220. H == 2 f1 lam,
-2.0106 × 1012 + 2.00532 × 1012 f1 + 2.02147 × 1012 fa - 1080. H - 58.32 H2 == 2 fa lam}
```

Solving for the variant fractions that minimize the energy as a function of applied field

```
fsol = Solve[simpeqns[H], {f1, fa}];
f1[H_, lam_] = f1 /. fsol[[1, 1]]
fa[H_, lam_] = fa /. fsol[[1, 2]]
-4.98672 × 10-13 (-2.0106 × 1012 - 1080. H - 58.32 H2) +
(4.98672 × 10-13 (2.00532 × 1012 (-1.99465 × 1012 - 1220. H) -
1. (-2.0106 × 1012 - 1080. H - 58.32 H2) (1.99063 × 1012 - 2. lam))
(2.02147 × 1012 - 2. lam)) / (-2.66948 × 1021 + 8.0242 × 1012 lam - 4. lam2)
- (1. (2.00532 × 1012 (-1.99465 × 1012 - 1220. H) -
1. (-2.0106 × 1012 - 1080. H - 58.32 H2) (1.99063 × 1012 - 2. lam)) /
(-2.66948 × 1021 + 8.0242 × 1012 lam - 4. lam2))
```

Solving for lambda

```

sol1 = Solve[f1[0, lam] == 2 / 3, lam]
sola = Solve[fa[0, lam] == 1 / 3, lam]
lambda = lam /. sola[[2]]

{{lam -> 1.15192 × 109}, {lam -> 5.08912 × 1011}}

{{lam -> -1.011 × 1012}, {lam -> 1.15033 × 109}}

1.15033 × 109

```

Checking the initial volume fraction distribution

```

f1[0, lambda]
fa[0, lambda]

0.666995

0.333333

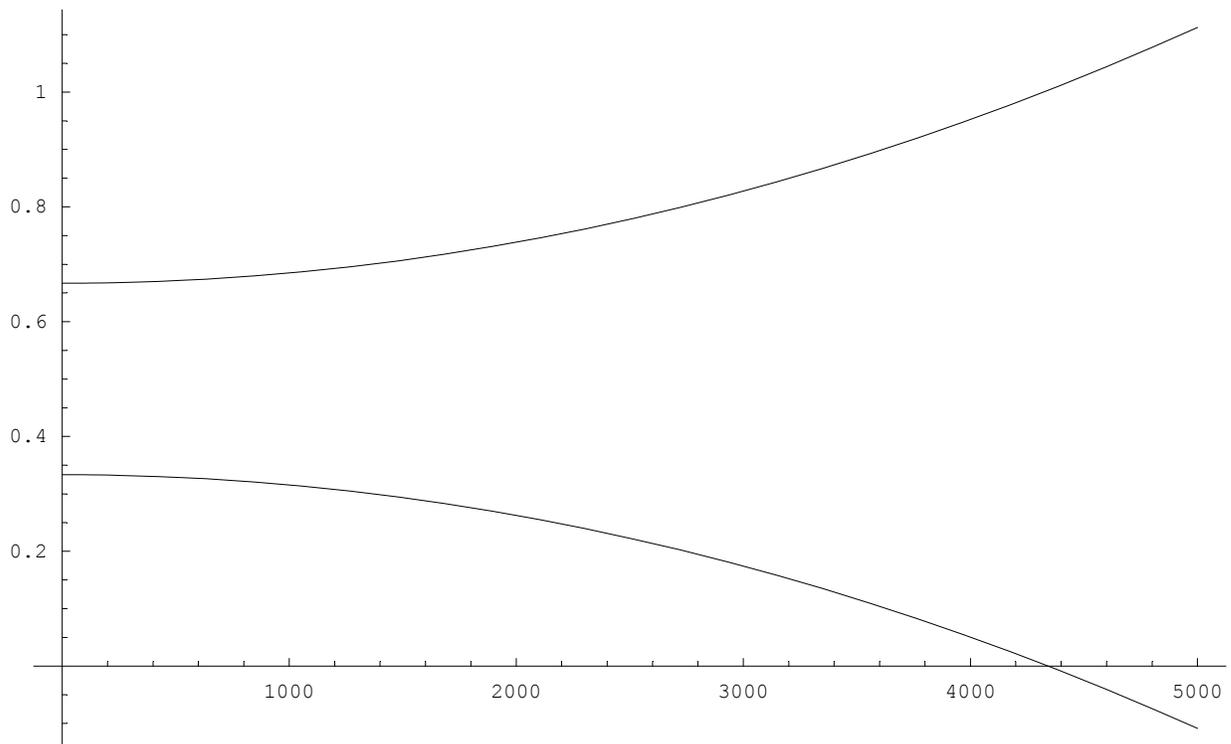
```

Volume fraction distribution vs. applied field

```

Plot[{f1[H, lambda], fa[H, lambda]}, {H, 1, 5000},
  AxesOrigin -> {0, 0}, AxesLabel -> {"H (kOe)", "f"}]

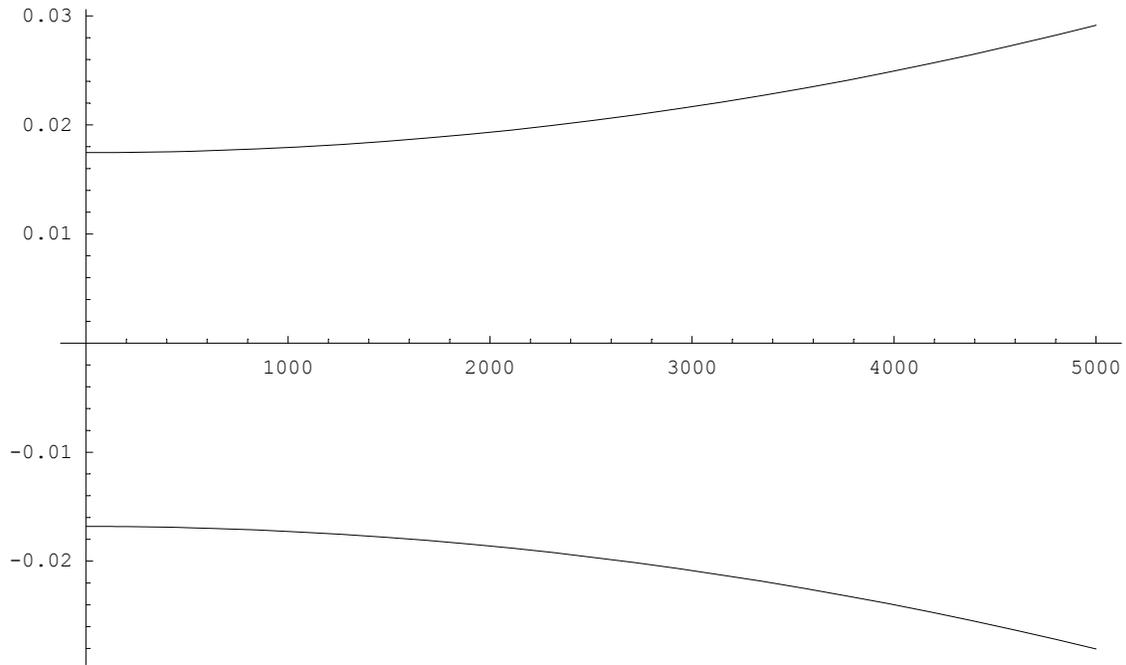
```



- Graphics -

Strain vs. applied field

```
exh[H_] =  
  ((f1[H, lambda] a + fa[H, lambda] ao) - (f1o a + f2o c + fao ao)) / (f1o a + f2o c + fao ao);  
eyh[H_] = ((f1[H, lambda] c + fa[H, lambda] ao) - (f1o c + f2o a + fao ao)) /  
  (f1o c + f2o a + fao ao);  
Plot[{exh[H], eyh[H]}, {H, 1, 5000}, AxesOrigin -> {0, 0}]
```



- Graphics -