Three-dimensional thermo-mechanical analysis of layered elastic/plastic solids

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Abstract

At high temperature a layered solid undergoes intense thermal loading that affects its mechanical performance. To study the thermo-mechanical behavior of a layered elastic/plastic solid, a three-dimensional numerical model based on the boundary element method (BEM) is developed. The thermal distortions and stresses are calculated with an arbitrary temperature field. The effect of temperature elevation on various failure mechanisms of the layered solid, such as plastic yielding, surface cracking, and layer/substrate delamination, are investigated. This BEM-based thermo-mechanical analysis is suitable for solids with large surface to volume ratio, such as shells and disks. An analysis is performed on magneto-optical media as a specific example. The result allows the specification of the thermo-mechanical properties of the media to alter the distributions of stresses and displacements without changing the temperature distribution. An optimal media design based on the simulation results is predicted.

1 Introduction

The fact that the coercivity of magnetic material drops at high temperatures allows thermally assisted magnetic recording with relatively weak magnetic fields. For example, magneto-optical (MO) recording is achieved by heating up the MO magnetic material near its Curie point temperature while applying a magnetic field. However, exposure to such a high temperature also subjects the MO media to an intense thermal loading, thus affecting its mechanical performance. For example, the temperature gradient and/or differences in thermo-mechanical properties of a layered structure may cause internal thermal distortions and thermal stresses. It is important that the only change to the media
when it is heated and cooled is the change in magnetization, with no damage to
the media itself. Therefore, a thermo-mechanical analysis, which predicts and
evaluates the mechanical performance under varying temperatures, is necessary.

2 BEM thermo-mechanical model

Analytical thermo-mechanical solutions are available for simple domains such as
semi-infinite solids [1]. For more complicated domains such as three-
dimensional layered elastic/plastic solids, an analytical solution is impossible and
alternative approaches are necessary. One approach is to discretize the boundary
of each layer into small elements so that numerical computation can be applied,
giving rise to the Boundary Element Method (BEM).

A Boundary Integral Equation (BIE) technique is applied here: governing
equations are expressed in integral equation forms (harmonic functions) over
each layer’s boundary. The 3-D thermo-elastic harmonic functions are
Boussinesq-Papkovich functions $\varphi$, $\psi_1$, and $\psi_3$ [2], which satisfy the following
harmonic equations

$$\nabla^2 \varphi = 2G \beta T, \quad \nabla^2 \psi_1 = \nabla^2 \psi_3 = 0, \quad \beta = \frac{\alpha(1+v)}{(1-v)}$$

where $G$ is the shear modulus, $v$ is Poisson’s ratio, and $\alpha$ is the coefficient of
thermal expansion.

The Fourier transform (represented by the symbol $\mathbb{F}$) is applied to expedite
the computation. The Boussinesq-Papkovich functions are then transferred from
the space domain into the frequency domain, and decomposed into sinusoids of
different frequencies:

$$\bar{\varphi} = A e^{-\rho z} + \bar{A} e^\rho z + \bar{\varphi}_T$$

$$\bar{\varphi}_T = \mathbb{F} \left[ \frac{-G \beta}{2\pi} \iiint_T \frac{T(x', y', z') dx' dy' dz'}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}} \right]$$

$$\bar{\psi}_1 = B e^{-\rho z} + \bar{B} e^\rho z$$

$$\bar{\psi}_3 = C e^{-\rho z} + \bar{C} e^\rho z$$

where the Fourier transform variables $\xi$ and $\eta$ correspond to $x$ and $y$,
respectively; and $\rho = \sqrt{\xi^2 + \eta^2}$. Since the governing equations throughout each
layer are expressed in integral equation forms over the layer boundary, applying
the boundary conditions solves the unknown factors $A$, $\bar{A}$, $B$, $\bar{B}$, $C$, $\bar{C}$. An
inverse Fourier transform then transfers the solutions from the frequency domain
back into the space domain.

Enforcing the equilibrium, compatibility, and Hooke’s law, the thermal
displacements and thermal stresses are given by

$$2Gu_i = \varphi_i + x\psi_{1,i} + z\psi_{3,i} - (3-4v)\psi_i$$

$$\sigma_{ij} = \varphi_{ij} - 2v(\psi_{1,i} + \psi_{3,i})\delta_{ij} - (1-2v)(\psi_{i,j} + \psi_{j,i}) + x\psi_{1,ij} + z\psi_{3,ij}$$

(3)
where the indices $i$ and $j$ range over 1, 2 and 3 corresponding to $x$, $y$ and $z$, respectively; and $\delta_{ij}$ is the Kronecker delta.

3 Results and discussion

3.1 BEM thermo-mechanical modeling of MO media

The BEM thermo-mechanical model is applied to MO media as an example. Figure 1 shows a typical quadrilayer-structured MO disk heated by a narrow laser beam while rotating. The temperature distribution within the disk is obtained from a sequentially-coupled electromagnetic/thermal conduction model [3, 4]. Since the temperature elevation zone is extremely small compared to the whole MO disk, the disk is considered as a layered half space and only the layers covered by the temperature elevation zone are modeled, i.e., the overcoat, magnetic layer, and intermediate layer. The reflector (Al) and substrate (PMMA) are merged into the intermediate layer since the temperature elevation is negligible in these layers. The magnetic layer (MnBi) is very thin compared to the adjacent layers and has a uniform temperature across its thickness, thus a membrane theory is applied to the magnetic layer so that the variation of the stress and strain across the thickness is neglected. The overcoat and the intermediate layer, both made of glass, have the following thermo-mechanical properties: elastic modulus = 73 GPa, coefficient of thermal expansion = 8.8 ($/C$), and Poisson’s ratio = 0.26.

Figure 1: (a) Schematic of MO recording, and (b) cross sectional contour of temperature in MO media.

The overcoat surface is stress-free provided that there is no head/media contact. Therefore, the boundary conditions at $z_1 = 0$ are given by:

\[
\sigma_{zz}^{(1)}(x, y, 0) = 0, \quad \sigma_{xz}^{(1)}(x, y, 0) = 0, \quad \sigma_{yz}^{(1)}(x, y, 0) = 0
\]

(4)

where the superscript (1) refers to the overcoat.
Both the overcoat and the intermediate layer are fully bonded to the magnetic layer. Since the magnetic layer functions as a membrane, the overcoat and the intermediate layer are required to have continuous stresses and displacements at their interfaces to the magnetic layer. Therefore, the interface condition at \( z_l = h \) and \( z_2 = 0 \) are given by

\[
\begin{align*}
\sigma_{xz}^{(1)}(x, y, h) &= \sigma_{xz}^{(2)}(x, y, 0) \quad u_x^{(1)}(x, y, h) = u_x^{(2)}(x, y, 0) \\
\sigma_{yz}^{(1)}(x, y, h) &= \sigma_{yz}^{(2)}(x, y, 0) \quad u_y^{(1)}(x, y, h) = u_y^{(2)}(x, y, 0) \\
\sigma_{zz}^{(1)}(x, y, h) &= \sigma_{zz}^{(2)}(x, y, 0) \quad u_z^{(1)}(x, y, h) = u_z^{(2)}(x, y, 0)
\end{align*}
\]

where the superscript \((2)\) refers to the intermediate layer and \( h \) is the overcoat thickness.

The stresses and displacements vanish into the substrate, i.e.,

\[
\begin{align*}
\sigma^{(2)}(x, y, \infty) &= 0, \quad u^{(2)}(x, y, \infty) = 0
\end{align*}
\]

The unknown factors \( A_i, A_7', B_i, E_i, C_i, \overline{C}_i, C_i \) \((i = 1, 2) \) are obtained by solving Eqns (4 – 6). The solution is the same as shown in a contact analysis \([5]\) with contact pressure \( P(x, y, 0) = 0 \) (see Appendix I), except that the following factors are complemented with additional thermal load terms:

\[
\begin{align*}
R_1 &= R_1 + \rho^{-1} \frac{\partial \Phi^{(1)}_{T,z}}{\partial z} \bigg|_{z=0} \\
R_2 &= R_2 - \rho^{-2} \frac{\partial \Phi^{(1)}_{T,z}}{\partial z} \bigg|_{z=0} \\
R_3 &= R_3 + \rho^{-1} e^{\rho h} \left( \Phi^{(1)}_{T,z} \bigg|_{z=h} - \Phi^{(2)}_{T,z} \bigg|_{z=0} \right) \\
R_4 &= R_4 + \rho^{-2} e^{\rho h} \left( -\Phi^{(1)}_{T,z} \bigg|_{z=h} + \Phi^{(2)}_{T,z} \bigg|_{z=0} \right) \\
R_5 &= R_5 + e^{\rho h} \left( -\Phi^{(1)}_T \bigg|_{z=h} + G \Phi^{(2)}_T \bigg|_{z=0} \right) \\
R_6 &= R_6 + \rho^{-1} e^{\rho h} \left( \Phi^{(1)}_{T,z} \bigg|_{z=h} - G \Phi^{(2)}_{T,z} \bigg|_{z=0} \right)
\end{align*}
\]

### 3.2 Thermo-mechanical performance of MO media

The thermal distortions and stresses occur simultaneously with the temperature elevation. Figure 2 shows the thermal distortions inside the MO disk. Large perpendicular thermal distortions (Fig. 2a) occur in the magnetic film and the intermediate layer. The maximum distortion coincides with the maximum temperature elevation. These distortions are the driving force for micro-displacement of the magnetic film, a potential source of cycle degradation. Along the radial direction (Fig. 2b), the thermal distortion is quite small and has negligible effect on the media performance.
The internal thermal stress may cause plastic yielding, surface cracking, delamination and ultimately media failure. For a ductile material such as the magnetic film, a major concern is the plastic yielding that occurs once the maximum von Mises stress exceeds its yielding strength. As shown in Fig. 3a, high von Mises stress occurs in the magnetic layer. The maximum value (0.14 GPa) coincides with the maximum temperature elevation and is far less than the plastic yield strength of most magnetic layers. For a brittle material such as glass, the major concern is surface ring cracking that occurs once the principal tensile stress exceeds the tensile strength. The radial principal tensile stress is shown in Fig. 3b, which turns out to be compressive at each layer surface so that surface ring cracking is unlikely to occur. However, repeated compressive stress can drive existing cracks to grow and break up into wear debris. The bonding failure of adjacent layers (delamination) is a major reliability concern in multilayered structures. The shear stress and the tensile stress at the layer/substrate interface are the major driving forces. As shown in Fig. 3c, relatively small shear stress at the interface can hardly break the bonding so that the shear adhesive failure of the interface (peel off delamination) is unlikely to occur. However, very high tensile stress, as shown in Fig. 3d, occurs right at the overcoat/magnetic layer/intermediate layer interface and the maximum value (0.17 GPa) coincides with the maximum temperature elevation. Therefore, it may break the bonding at that location and generate a crack. High tensile stresses around, serving as a crack driving force, may then help the crack to grow and eventually lead to the adhesive failure of the interface (pull off delamination).
Figure 3: Contours of thermal stress in MO media, (a) von Mises stress $J^{1/2}$, (b) radial principal tensile stress $\sigma_r$, (c) shear stress component $\sigma_{xz}$, and (d) tensile stress component $\sigma_{zz}$.

To avoid these potential thermal-induced media failures, the thermal distortions and thermal stresses need to be carefully controlled. The comparison between Fig. 1 and Figs. 2 and 3 shows that the distributions of the thermal stresses and distortions are largely determined by the temperature distribution. For example, the maximum perpendicular distortions, perpendicular stress, and von Mises stress coincide with the maximum temperature elevation. Since the temperature distribution is required for thermally assisted recording and is therefore fixed, so are the distributions of thermal distortions and stresses. Optimizing the thermo-mechanical properties of the media, however, can still reduce the magnitudes of the maximum thermal stresses and distortions. A parametric study is performed based on the same temperature distribution but varying thermo-mechanical properties of the overcoat. As shown in Fig. 4a, choosing an overcoat with smaller elastic modulus, relative to the intermediate layer, reduces the maximum perpendicular thermal distortion. An overcoat with matching coefficients of thermal expansion to the intermediate layer, i.e., $\alpha_1/\alpha_2 \sim 1$, generates the minimum distortion. The maximum thermal von Mises stress, as shown in Fig. 4b, is reduced with an overcoat with smaller elastic modulus and coefficient of thermal expansion.
Figure 4: Variation of (a) the maximum perpendicular distortion $u_{z_{max}}$ and (b) the maximum von Mises stress $J^{1/2}$ with the elastic modulus $E_i$ and coefficients of thermal expansion $\alpha_i$ of the overcoat ($i = 1$) and the intermediate layer ($i = 2$).

3.3 Benchmark test of the thermo-mechanical model: Boundary Element method vs. Finite Element method

This BEM thermo-mechanical model has been benchmarked with a commercially available Finite Element package (ANSYS/Mechanical). The results of these two models are consistent. Since ANSYS does not have infinite boundary elements for structural analysis [6], a finite 3D volume containing the temperature elevation zone has been modeled and meshed. Due to the number limit and aspect ratio requirement of finite elements, the volume can only cover a limited portion of the MO disk, which is a modeling deficiency. In BEM, the entire MO disk is modeled as an infinite half space. Since the integral equation form is used in the computation, only the surface of the elevated temperature zone needs to be meshed. Therefore, the BEM approach is substantially easier to use than finite element and finite difference methods, especially for the analysis with shapes that have a large surface to volume ratio, such as shells and disks, where the aspect ratio requirement is very stringent.

4 Conclusions

A BEM thermo-mechanical model is developed to calculate the thermal distortions and stresses under given temperature distributions. This model is applied to MO media as a specific example. The major potential failure modes are the micro-displacement of the magnetic film and the pull off delamination at the magnetic layer/intermediate layer interface. The maximum thermal stresses and distortions are reduced by optimizing the layer/substrate design without
changing the temperature distribution. This BEM model is benchmarked with a commercial available FEM model and shows its advantage in modeling disk structures.

Acknowledgement

This work was performed under the support of the U. S. Department of Commerce, National Institute of Standards and Technology, Advanced Technology Program, Cooperative Agreement Number 70NANB1H3056.

References


Appendix I: solutions of the terms $A^{(i)}$, $\overline{A}^{(i)}$, $B^{(i)}$, $\overline{B}^{(i)}$, $C^{(i)}$, $\overline{C}^{(i)}$ ($i = 1, 2$)

Defining the terms $G_1$, $G_2$, $G$, $\lambda$, $k$, and $S_0$ by

$$G_1 = \frac{E_1}{2(1+\nu_1)}, \quad G_2 = \frac{E_2}{2(1+\nu_2)}, \quad G = \frac{G_1}{G_2}$$

$$\lambda = 1 - \frac{4(1-\nu_1)}{1 + G(3-4\nu_2)}$$

$$k = \frac{G-1}{G + (3-4\nu_1)}$$

$$S_0 = [G + (3-4\nu_1)][1 - ke^{-2\alpha h}]$$

the terms $B^{(1)}$, $\overline{B}^{(1)}$, $B^{(2)}$, and $\overline{B}^{(2)}$ are given by

$$\overline{B}^{(1)} = \frac{(G-1)e^{-2\rho h}}{(1+G)+(1-G)e^{-2\rho h}} \mu \frac{\overline{p}(\xi, \eta, 0)}{2\rho(1-\nu_1)}$$

$$B^{(1)} = \overline{B}^{(1)} + \frac{\mu \overline{p}(\xi, \eta, 0)}{2\rho(1-\nu_1)}$$

$$B^{(2)} = 2(1-\nu_1)\frac{e^{-\rho h}}{1-\nu_2} \frac{(1+G)+(1-G)e^{-2\rho h}}{(1+G)+(1-G)e^{-2\rho h}} \mu \frac{\overline{p}(\xi, \eta, 0)}{2\rho(1-\nu_1)}$$

$$\overline{B}^{(2)} = 0$$

where $\overline{p}(\xi, \eta, 0)$ is the Fourier transform of $p(x, y, 0)$. 

Defining the terms $R_1, R_2, R_3, R_4, R_5$ and $R_6$ by

\[-\rho^2 R_1 = i\xi \ (B^{(1)} - \overline{B}^{(1)} ) + i\rho^2 (B_{\xi}^{(1)} - \overline{B}_{\xi}^{(1)}) \]

\[-\rho^2 R_2 = 2i\xi \ (1-\nu_1) (B^{(1)} + \overline{B}^{(1)}) + i\rho^2 (B_{\xi}^{(1)} + \overline{B}_{\xi}^{(1)}) + \overline{p}(\xi , \eta, 0) \]

\[-\rho^2 R_3 = i(\xi - \xi \rho h) B^{(1)} - i(\xi + \xi \rho h) e^{2\rho h \overline{B}^{(1)}} - i\xi e^{\rho h B^{(2)}} \]

\[+ i\rho^2 B_{\xi}^{(1)} - i\rho^2 e^{2\rho h \overline{B}_{\xi}^{(1)}} - i\rho^2 e^{\rho h B_{\xi}^{(2)}} \]

\[-\rho^2 R_4 = [2i(1-\nu_1)\xi - i\xi \rho h] B^{(1)} + [2i(1-\nu_1)\xi + i\xi \rho h] e^{2\rho h \overline{B}^{(1)}} \]

\[-[2i(1-\nu_2)\xi] e^{\rho h B^{(2)}} + i\rho^2 B_{\xi}^{(1)} + i\rho^2 e^{2\rho h \overline{B}_{\xi}^{(1)}} - i\rho^2 e^{\rho h B_{\xi}^{(2)}} \]

\[-\rho^2 R_5 = -i\xi \rho h B^{(1)} + i\xi \rho h e^{2\rho h \overline{B}^{(1)}} + i\rho^2 B_{\xi}^{(1)} + i\rho^2 e^{2\rho h \overline{B}_{\xi}^{(1)}} \]

\[-iG \rho^2 e^{\rho h B_{\xi}^{(2)}} \]

\[-\rho^2 R_6 = i(\xi - \xi \rho h) B^{(1)} - i(\xi + \xi \rho h) e^{2\rho h \overline{B}^{(1)}} - i\xi e^{\rho h B^{(2)}} \]

\[+ i\rho^2 B_{\xi}^{(1)} - i\rho^2 e^{2\rho h \overline{B}_{\xi}^{(1)}} - iG \rho^2 e^{\rho h B_{\xi}^{(2)}} \]

and defining the terms $R_a, R_b, R_c$ and $R_d$ by

\[R_a = (G-1)\rho(R_1 + R_2) - G\rho(R_3 + R_4) + \rho(R_5 + R_6) \]

\[R_b = \rho(R_2 - R_1) + \rho e^{-2\rho h}(R_3 - R_4) \]

\[R_c = \frac{4(1-\nu_1)}{1-\lambda} \frac{2\rho h e^{-2\rho h}}{S_0} R_a + R_b \]

\[R_d = \rho[R_1 - R_2 - R_3 + R_4] + \frac{(1-\lambda)\rho}{4(1-\nu_1)} (R_3 - R_4 + R_5 - R_6) \]

the terms $A^{(1)}, \overline{A}^{(1)}, C^{(1)}, \overline{C}^{(1)}, A^{(2)},$ and $C^{(2)}$ are given by

\[C^{(1)} = (1-\lambda)k S_0 R_c / \{4(1-\nu_1)(G-1)[1-(\lambda + k + 4k \rho^2 h^2)e^{-2\rho h} \]

\[+ \lambda k e^{-4\rho h}] \}

\[\overline{C}^{(1)} = \{2(G-1)\rho h e^{-2\rho h} C^{(1)} + e^{-2\rho h} R_a \} / S_0 \]

\[A^{(1)} = \{-3 - 4\nu_1\} C^{(1)} + C^{(1)} + \rho(R_1 + R_2)\} / (2\rho) \]

\[\overline{A}^{(1)} = \{(1-\lambda)e^{-2\rho h} C^{(1)} + [(3-4\nu_1)(1-e^{-2\rho h}) - 2\rho h]\overline{C}^{(1)} + e^{-2\rho h} R_d \}

\[l / [2\rho(1-e^{-2\rho h})] \]

\[C^{(2)} = \{[4(1-\nu_1)(1-\lambda)e^{-\rho h}] C^{(1)} + (1-\lambda)\rho e^{-\rho h} [R_3 - R_4 + R_5 - R_6] \}

\[l / [4(1-\nu_1)] \]

\[A^{(2)} = \{2\rho h e^{-\rho h} [S_0 - (G-1)(1-e^{-2\rho h})] C^{(1)} - [(3-4\nu_2)S_0] C^{(2)} + \]

\[\rho e^{-\rho h} S_0 (R_1 + R_2 - R_3 - R_4) - e^{-\rho h} (1-e^{-2\rho h}) R_a \} / (2\rho S_0) \]

\[\overline{C}^{(2)} = 0 \]