Thermal Residual Stresses in Eutectic Composites

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Outline

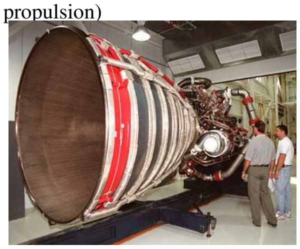
1. Introduction
2. Analytical Solutions
3. FEM with ANSYS
4. Compare Solutions

Introduction

- Potential Applications
- Directionally Solidified Eutectic System
- Microstructure of DSE System
- Material Properties of DSE System
- Goals and Objectives
  - Understand Thermal Residual Stresses

Potential Applications

- ☐ New candidates for ultra-high temperature materials (UHTMs)
- ☐ Heat engines used in aerospace shuttles
- ☐ Used in extreme environments (above 3000℃ during rocket propulsion)



The upgraded Block 2 engine sits in the Space Shuttle Main Engine Processing Facility at Kennedy Space Center awaiting transfer to Atlantis' hangar

Space Shuttle Main Engine (SSME) Test Firing from NASA

Directionally Solidified Eutectic System

LaB_6-ZrB_2 eutectic system phase diagram

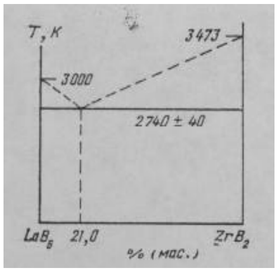


Figure 1:The phase diagram indicates an ultra-high eutectic temperature (2740K) of the LaB6-ZrB2 system and no intermediate phases were formed

Ordanyan, Paderno et al. 1983

Crystal Structure of LaB_6-ZrB_2

LaB_6 unit cell

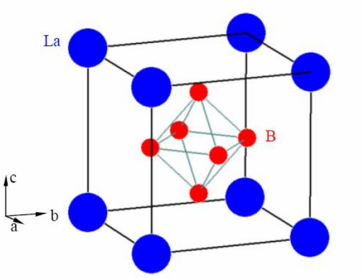


Figure 2: Model of the LaB_6 unit cell, which has the CaB_6-structure [adapted from Wyckoff and Ralph 1986].

ZrB_2 unit cell

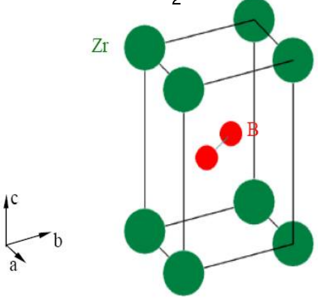


Figure 3: Model of the unit cell of ZrB_2 presents a AlB_2 structure [adapted from Wyckoff and Ralph 1986].

Wycoff and Ralph 1986

Microstructure of LaB_6-ZrB_2

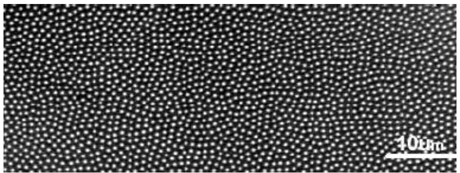


Figure 4: Optical micrograph showing the microstructure of LaB_6-ZrB_2, in which ZrB_2 fibers (white) distribute throughout the LaB_6 matrix (dark) uniformly

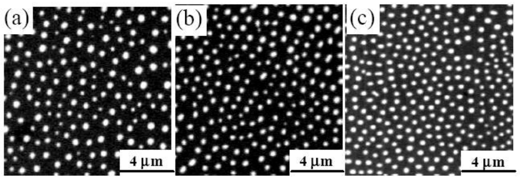
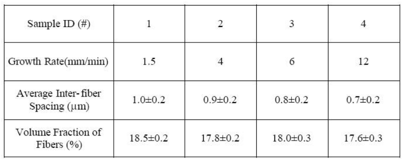


Figure 5: Optical micrographs of the transverse sections of (a) sample #1 (grown at a speed of 1.5mm/min), (b) sample #2 (grown at a speed of 1.5mm/min) and (c) sample #4 (grown at a speed of 1.5mm/min).

Microstructure of LaB_6-ZrB_2

Measured Values of Inter-fiber Spacing and Volume Fractions



Sample ID (#)	1	2	3	4
Growth Rate(mm/min)	1.5	4	6	12
Average Inter-fiber Spacing (μm)	1.0±0.2	0.9±0.2	0.8±0.2	0.7±0.2
Volume Fraction of Fibers (%)	18.5±0.2	17.8±0.2	18.0±0.3	17.6±0.3

Figure 7: Measured average spacing between fibers and the volume fractions of fibers from sample #1, #2, #3 and #4.

Inter-fiber Spacing λ, and Growth Rate R

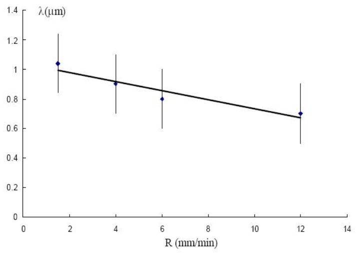


Figure **8**: Relationship between the inter-fiber spacing λ and the growth rate R.

Material Properties of LaB_6-ZrB_2

- The 2nd order thermal expansion coefficient (CTE) tensors of LaB6 and ZrB2 are isotropic and orthotropic, respectively. Because of their dependence on temperature, the coefficients are represented as functions of temperature

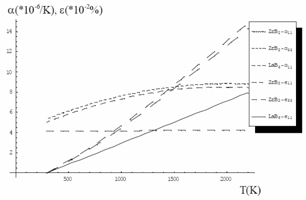


Figure 9: Plot of the CTEs and thermal expansions vs. temperature for LaB_6 and ZrB_2 [TPRC 1970; Bonstein 2005].

Other Material Properties

	Te (°C)	Microhardness (GPa)	Fracture Toughness ($MPa \cdot m^{1/2}$)	Strength (MPa)
LaB_6-ZrB_2	2467± 40 [Ordanyan, Paderno et al. 1983]	25.50 [Ordanyan, Paderno et al. 1983]	20.3~27.8 [Ordanyan, Paderno et al. 1983]	1000~1320 [Ordanyan, Paderno et al. 1983]

Figure 10: Some Mechanical Properties of the System

Goals and Objectives

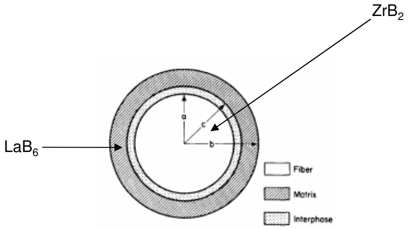
- Understand Thermal Residual Stresses
  - Thermal residual stresses result from a good bonded interface and thermal expansion mismatch between LaB_6 and ZrB_2

- Model Thermal Residual Stresses in DSE LaB_6-ZrB_2
  - Analytical Solutions
  - FEM using ANSYS

- Compare Solutions
  - ANSYS vs. XRD

Analytical Solutions

Isotropic Fiber/Matrix Composite Model



a = radius of fiber = 2.88µm
b = radius of matrix = 7.04µm
c = a (the volume fraction of the interphase is zero)

Figure 11 shows cross-section of cylinder model for undirectional composite

Nairn, J. "Thermoelastic Analysis of Residual Stresses in Undirectional, High-Performance Composites". Central Research and Development E.I. DuPont de Nemours Co. Polymer Composites, April, 1985, Vol. 6, No. 2

Analytical Solutions

- Equations for LaB$_6$ (Cubic System)

Shear Modulus → $G = 1/5(C_{11}-C_{12}+3C_{44})$

Bulk Modulus → $B = (C_{11}+2C_{22})(1/3)$

Young's Modulus → $E = G\left(\frac{3B}{B+1/3\,G}\right)$

Poisson's Ratio → $\nu = \left(\frac{B - 2/3\,G}{2\left(B+1/3\,G\right)}\right)$

- Sample Calculations for LaB$_6$

→$G = 1/5(453.3 - 18.2 + 3(90.1)) = 141.08$ GPa

→$B = (453.3 + 2(18.2))(1/3) = 163.23$ GPa

→$E = 141.08[(3*163.22)/(163.22 + 1/3(141.08))]$
$= 328.57$ GPa

→$\nu = (163.22 - 2/3(141.08))/2(163.22 + 141.08/3)$
$= 0.1645$

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Analytical Solutions

ZrB_2 Fiber

E_f = 424 GPa
υ_f = 0.150
α_f = 6.8x10-6(K-1)
V_f = 0.277

Fiber Elastic Constants
C_{11} = 567.8 GPa
C_{12} = 56.9 GPa
C_{13} = 120.5 GPa
C_{33} = 436.1 GPa
C_{44} = 247.5 GPa

Bornstein, Second and Higher Order Elastic Constants

LaB_6 Matrix

E_m = 328GPa
υ_m = 0.1654
α_m = 6.7x10-6(K-1)
V_m = 0.723

Matrix Elastic Constants
C_{11} = 453.3 GPa
C_{12} = 18.2 GPa
C_{44} = 90.1 GPa

Bornstein, Second and Higher Order Elastic Constants

Analytical Solutions

Calculating the A parameters

$$A_{11} = 2\left(\frac{\upsilon_m}{E_m} + \frac{\upsilon_f}{E_f} + \frac{v_m}{v_m}\right)$$

$$A_{12} = -\left(\frac{v_m}{E_f v_f} + \frac{1}{E_m}\right)$$

$$A_{21} = -\left(\frac{(1 - v_f)\, v_m}{E_f v_f} + \frac{(1 - \upsilon_m)}{E_m} + \frac{(1 + \upsilon_m)}{E_m v_f}\right)$$

$$A_{22} = \left(\frac{A_{11}}{2}\right)$$

$$A_3 = \left(\frac{A_{21} \bullet \Delta\alpha_L - A_{11} \bullet \Delta\alpha_T}{A_{21} \bullet A_{12} - A_{11} \bullet A_{22}}\right)\Delta T$$

$$A_1 = \left(\frac{\Delta\alpha_L \bullet T - A_{12} \bullet A_3}{A_{11}}\right)\Delta T$$

$$A_2 = -b^2 A_1$$

$$A_7 = A_1\left(\frac{a^2 - b^2}{b^2}\right)$$

$$A_8 = A_3\left(\frac{a^2 - b^2}{b^2}\right)$$

Sample Calculations

A_{11} = 2.851*10^{-3} (GPa^{-1})

$\Delta\alpha_L$ = -0.17*10^{-6}
$\Delta\alpha_T$ = -0.17*10^{-6}

A_{12} = -9.129*10^{-3} (GPa^{-1})

A_{21} = -20.571*10^{-3} (GPa^{-1})

A_{22} = 1.426*10^{-3} (GPa^{-1})

A_3 = -104.090 (MPa)

A_1 = -335.454 (MPa)

A_2 = 166.256^3 (MPa*m^2)
A_7 = 1,668.987 (MPa)
A_8 = 517.880 (MPa)
Δt = (Eutectic Temp. to Room Temp:
2740K → 300K) = -2440K

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Analytical Solutions

- ☐ Final Solution

Matrix LaB_6 (compression)

$\sigma_r = A_1 + \left(\frac{A_2}{r^2}\right)$ $\sigma_r = -335.454 + 166.256/r^2$

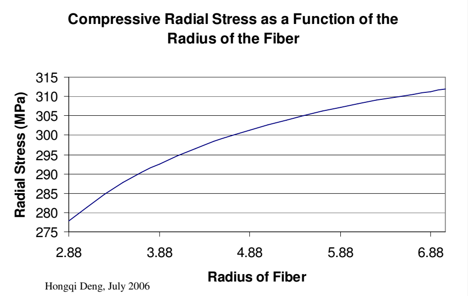
$\sigma_z = A_3$ $\sigma_z = -104.090$ (MPa)

Fiber ZrB_2 (tension)

$\sigma_r = A_7$ $\sigma_r = 1.669$ (GPa)

$\sigma_z = A_8$ $\sigma_z = 517.880$ (MPa)

Subscript r means radial,
likewise z means axial



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ANSYS Solutions

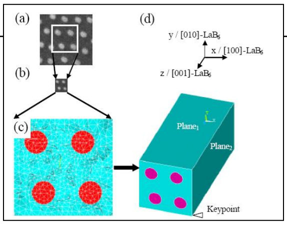

Figure 12 : (b) A structure unit from (a) the SEM micrograph of the actual microstructure on the transverse section was used to create (c) the two-dimensional model, which was extruded along the *z* direction to create (d) the three-dimensional model based on the data representing frame (x, y, z)

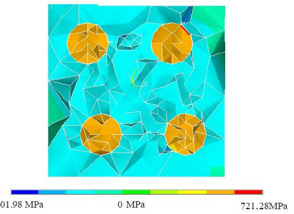

Figure **13**: Contour plot of the axial stress σ_{zz}, the stress along the fiber- matrix interface.

Assume stress free temperature equal to 2740 K:

$$\sigma_{ZrB_2} = \begin{bmatrix} 990.5 & -1.094 & -17.01 \\ -1.094 & 908.7 & -23.49 \\ -17.01 & -23.49 & 649.6 \end{bmatrix} \text{MPa}$$

$$\sigma_{LaB_6} = \begin{bmatrix} -200.0 & -6.5 & -5.1 \\ -6.5 & -195.3 & -0.91 \\ -5.1 & -0.91 & -142.6 \end{bmatrix} \text{MPa}$$

Assume stress free temperature equal to 2400 K:

$$\sigma_{ZrB_2} = \begin{bmatrix} 714.8 & -4.092 & -6.290 \\ -4.092 & 622.0 & -8.450 \\ -6.290 & -8.450 & 530.6 \end{bmatrix} \text{MPa}$$

$$\sigma_{LaB_6} = \begin{bmatrix} -139.2 & -1.4 & -5.6 \\ -1.4 & -137.6 & -0.81 \\ -5.6 & -0.81 & -116.5 \end{bmatrix} \text{MPa}$$

	Elastic Constants (GPa)						Thermal expansion strain ($*10^{-3}$)			
	E_x	E_y	E_z	ν_{xy}	G	μ_{yz}		300K	2400K	2740K
LaB_6	451.9	451.9	451.9	0.0386	163.6	90.1		0	8.823	10.273
ZrB_2	533.5	533.5	389.6	0.2641	240.2	247.5	//[100]	0	16.542	19.409
							//[001]	0	15.921	18.681

Constants of the LaB_6 and ZrB_2 used in FEM [TPRC 1970; Tanaka, Yoshimoto et al. 1977; Okamoto, Kusakari et al. 2003; Bonstein 2005

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Comparison of XRD Results and FEM using ANSYS

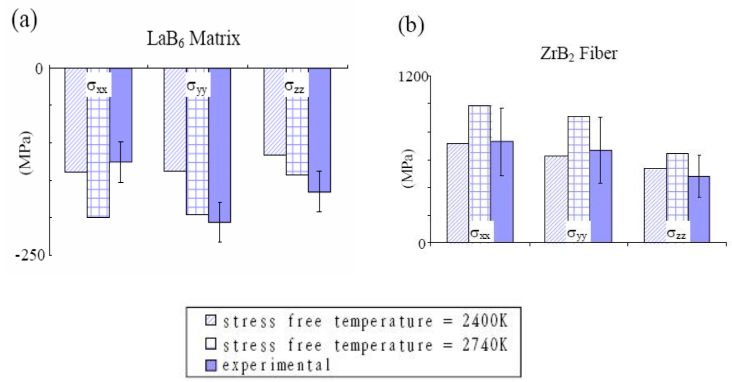

Figure **14**: Plot of XRD and FEM results for (a) the matrix and (b) fibers.

Comparison of XRD Results and FEM using ANSYS

- □ Most stress components of the FEM data (under 2740 K stress-free temperature) higher than XRD
- □ Stresses at 2400 K stress-free temperature assumption agree with the XRD results for the fiber phase, but lower than the XRD for the matrix
- □ It seems at 2400 K, 87% of the eutectic temperature, is a better approach for estimating the stress free temperature than 2740 K
- □ The absolute answer of the stress free temperature requires XRD measurements at a series of temperatures.

Future Work

- Use OOF to model thermal residual stresses in DSE LaB_6-ZrB_2
- Compare OOF solutions to ANYS solutions
- Model thermal residual stresses in pseudo-binary eutectic composites