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REACTIVE NANO-FILMS OF AL AND PT

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5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)

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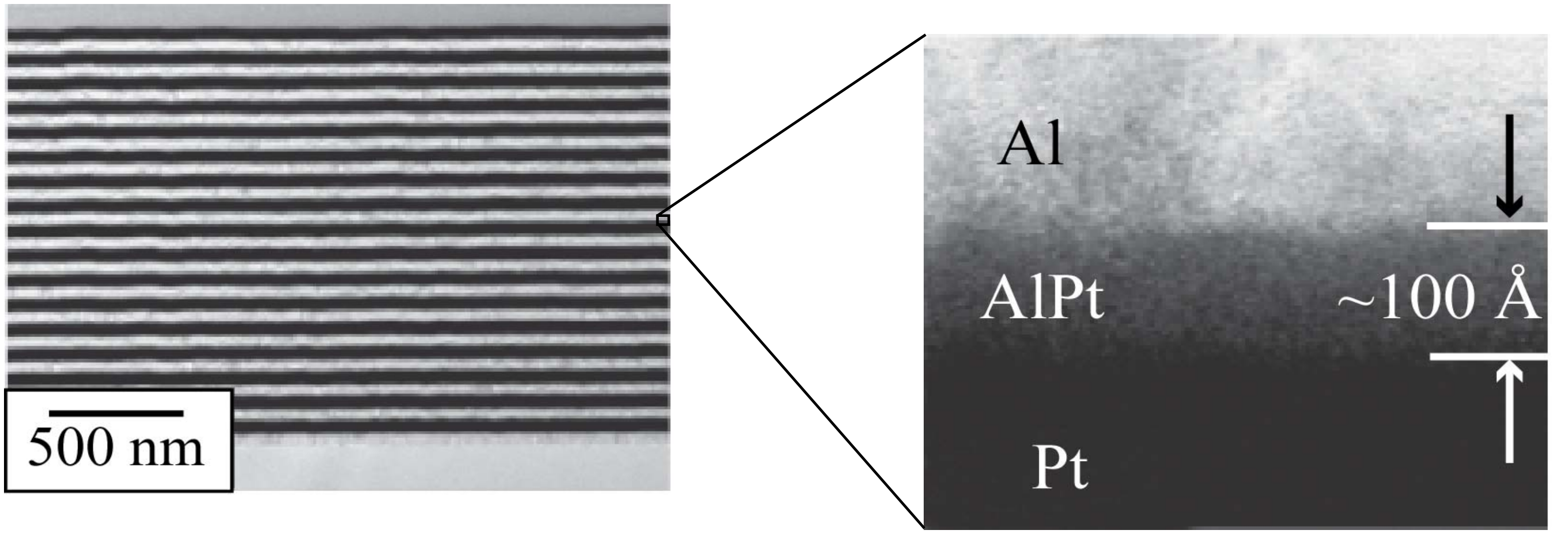
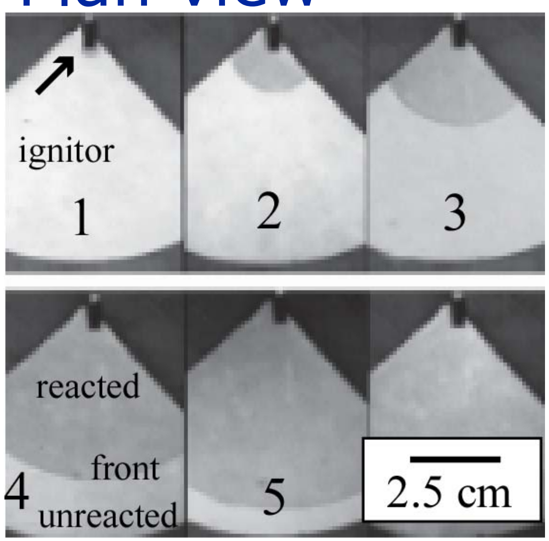
Soldering or Brazing of Microelectronics
(Rapid, localized heating minimizes damage)

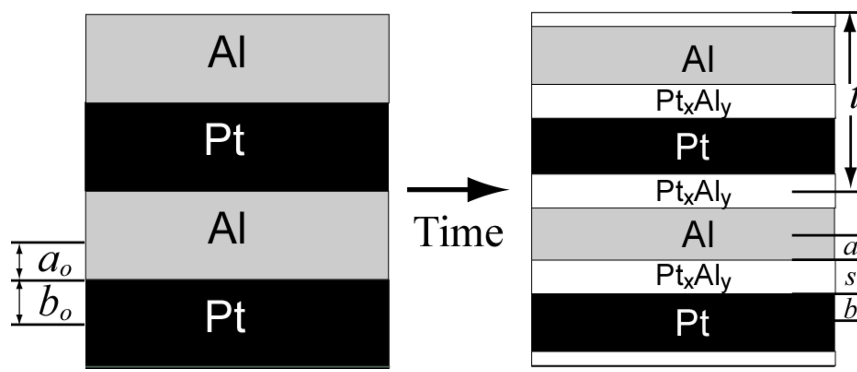
Cross section



Plan view



Schematic



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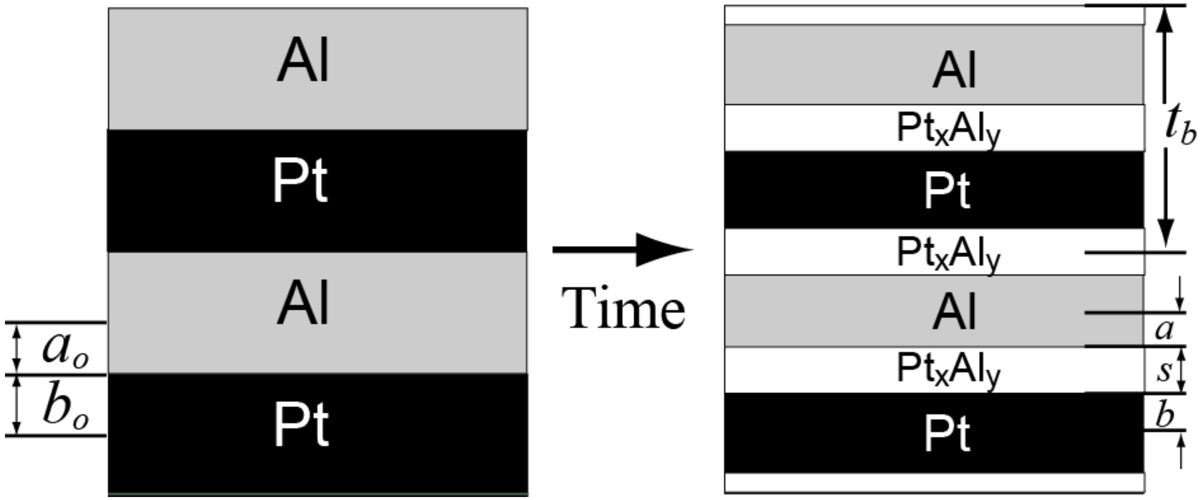
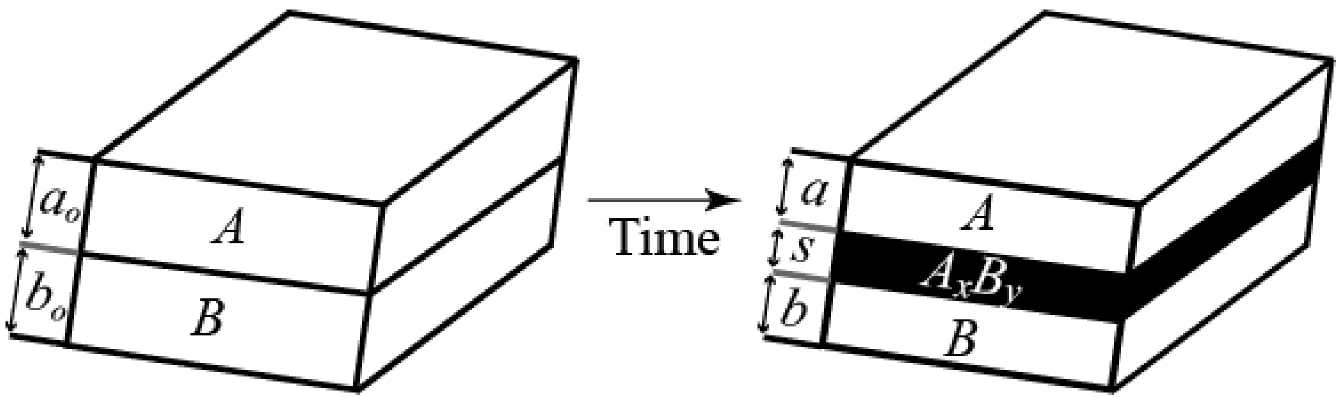
Two bilayers of Al and Pt





$$t_b = 2(a + b + s)$$

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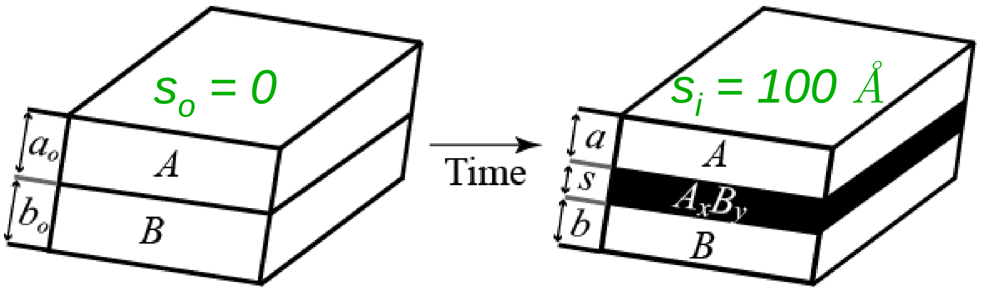
1D diffusion controlled growth reaction with zero strain assumption*



$$\xi_A A + \xi_B B \rightarrow A_{\xi_A} B_{\xi_B} + Q$$

ODE's

$$\frac{da}{dt} = -\frac{D}{s}$$

$$\frac{db}{dt} = -\frac{b_o}{a_o}\frac{D}{s}$$

$$\frac{ds}{dt} = -\frac{D}{s}\left(1+\frac{b_o}{a_o}\right)$$

$$\frac{dF}{dt} = -\frac{D}{a_o s}$$

Auxiliary Eqns.

$$D = D_o \exp(-\tfrac{E}{RT})$$

$$a = \frac{a_o + b_o - s}{1 - \frac{\rho_A}{\rho_B}\frac{M_B}{M_A}\frac{\xi_B}{\xi_A}}$$

$$b = a\frac{\rho_A}{\rho_B}\frac{M_B}{M_A}\frac{\xi_B}{\xi_A}$$

$$\rho_{AB} = \frac{a_o\rho_A + b_o\rho_B}{a_o + b_o}$$

Algorithm

Choose a_o, calculate b_o

Choose s_i, calculate a_i, b_i, and F_i

Solve ODE's for s and F

Energy Equation

$$\rho c\frac{\partial T}{\partial t}\nabla\cdot(k\nabla T) = -Q\rho\frac{dF}{dt}$$

*Hardt AP and Phung PV, "Propagation of gasless reactions in solids—I. Analytical study of exothermic intermetallic reaction rates," *Combustion and Flame*, **21**, pp. 77-89, 1973.

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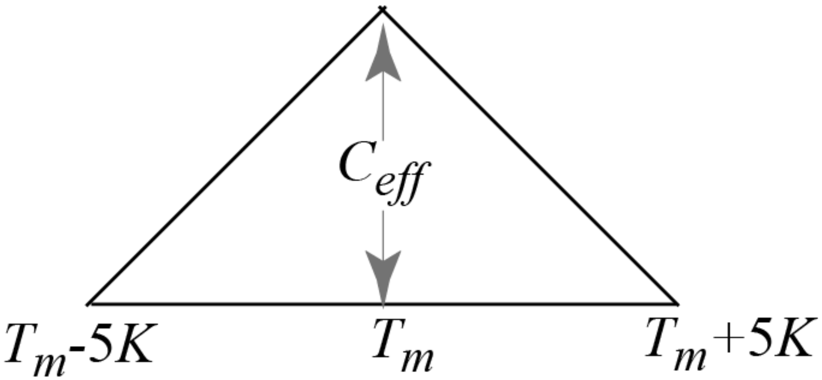
Parameters

Thermophysical Properties

Property	Description	Al	Pt	AlPt
c, J/kgK	Specific Heat	894-900	133	226
c_{eff}, J/kgK	Effective c at T_m	h_{fus}/° T	h_{fus}/° T	h_{fus}/° T
° T, K	half of mush zone	4-6	4-6	4-6
h_f, J/kg	Formation enthalpy	0	0	-901,000
h_{fus}, J/kg[b]	Latent enthalpy	397,000	114,000	48,300; 100,000
k, W/mK	Thermal conductivity	213-261	71.6	158
M_w, kg/kgmol	Molecular weight	27.0	195	222
°, kg/m^3	Density	2700	21500	11600
T_m, K	Melting point	934	2040	934, 2040

Diffusion model parameters

Property	Description	AlPt
s_o, m	Initial thickness of reacted layer	1×10^{-8}
D_o, m^2/s	Initial diffusion coefficient	1×10^{-7}
E, J/kgmol	Activation energy	4.1868×10^{7}



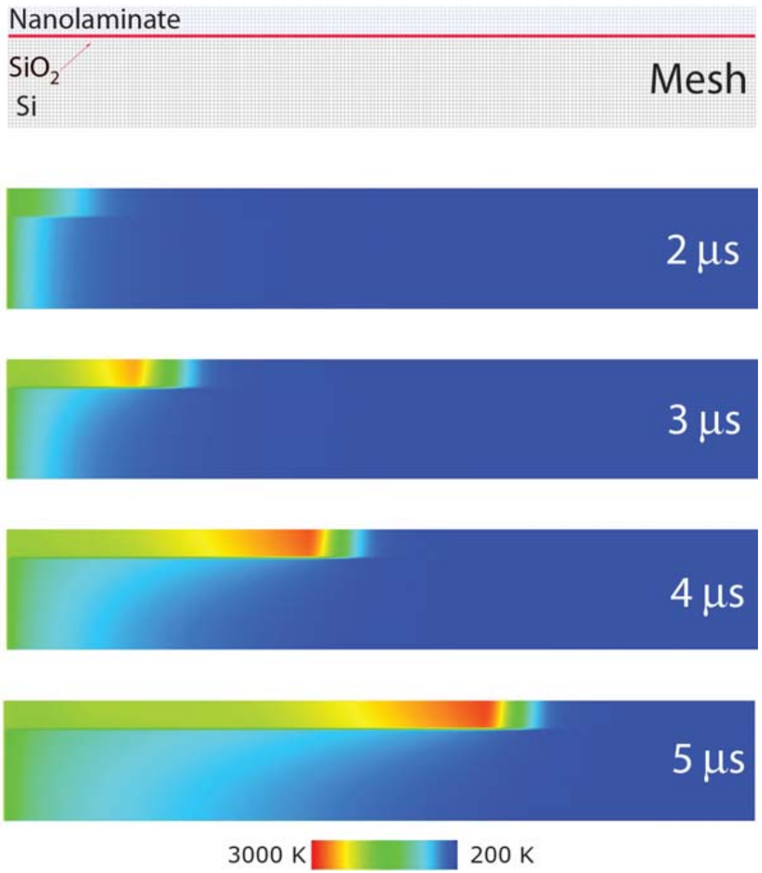
$$Area = ½(Base \times Height)$$
$$h_{fus} = ½(10\ \mathrm{K} \times C_{T_{mp}})$$
$$C_{T_{mp}} = 5 \times h_{fus}$$

Two Phase Changes (Al, Pt)*

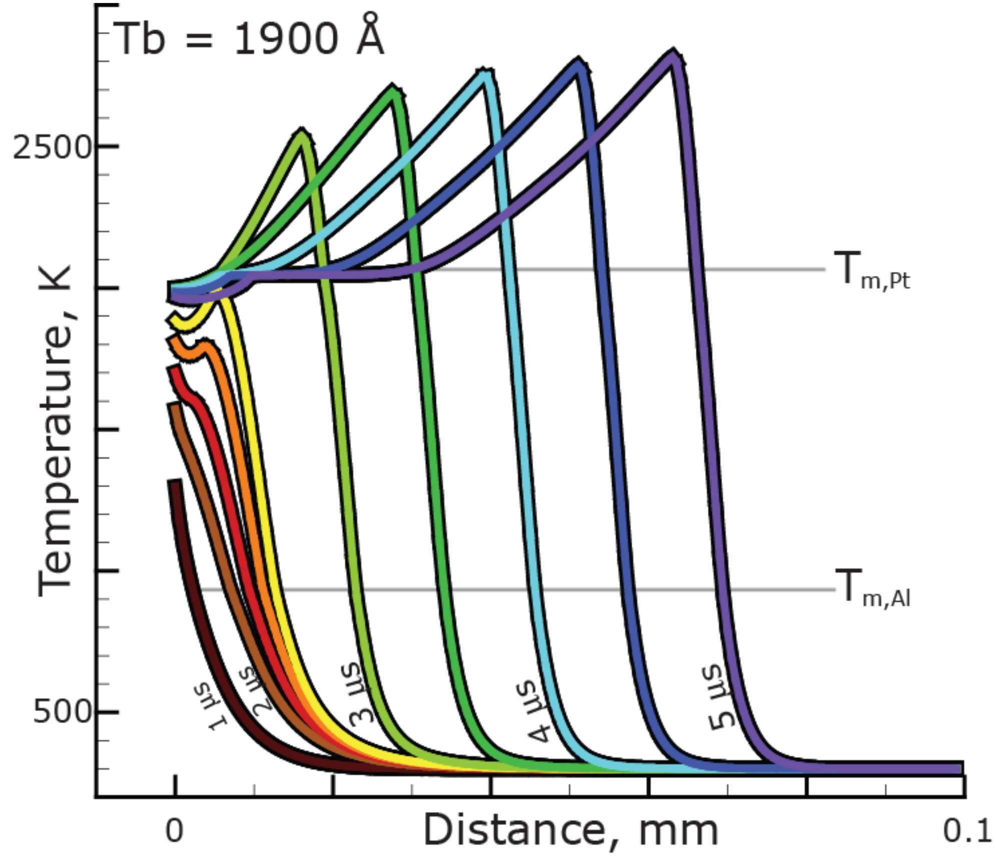
*Effective capacitance method: Yao, L.S. and Prusa, J., Melting and freezing, *Advances in Heat Transfer*, 5th Edition, John Wiley & Sons, New York, 2002.

Temperature profiles leading to ignition

2D Axisymmetric Temperature



Temperature on top of nanolaminate



Reaction energy sufficient to melt both layers

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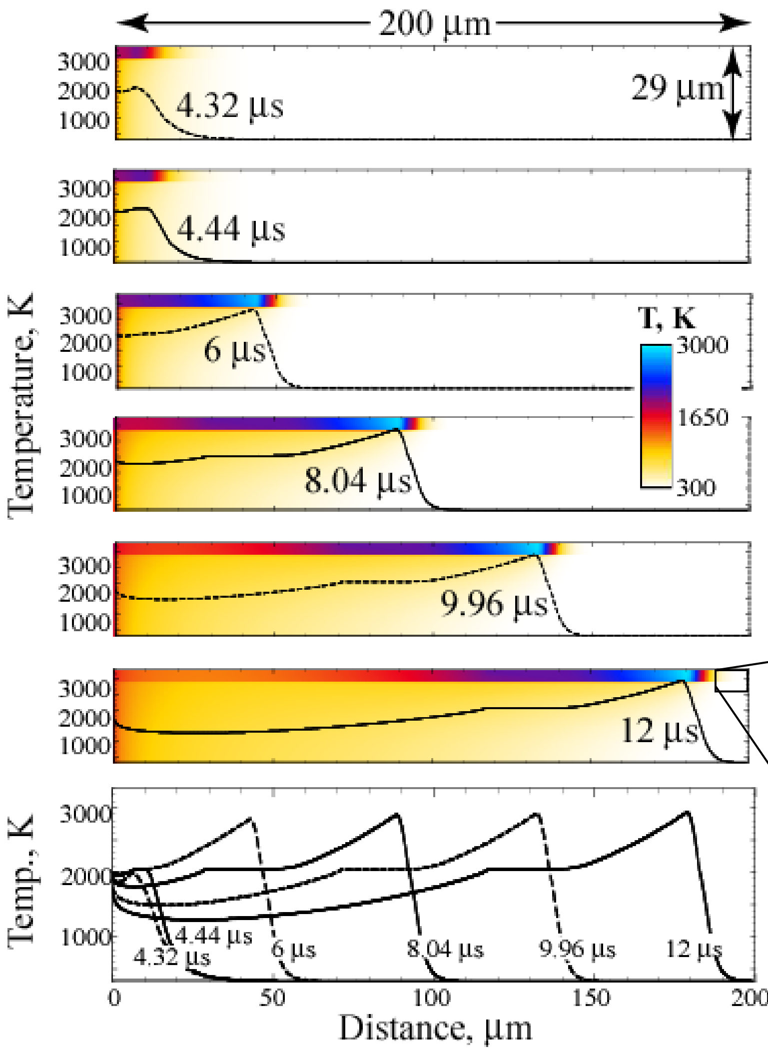
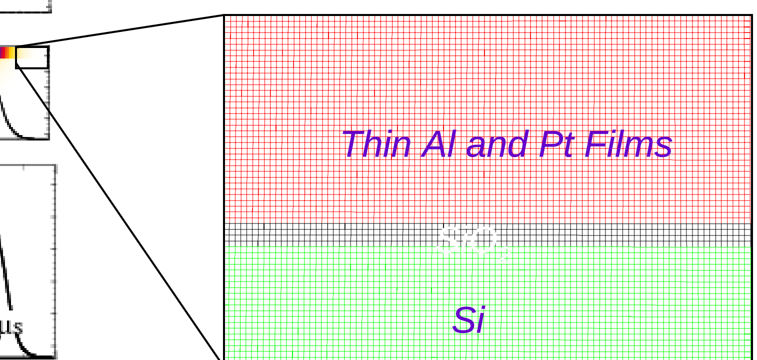
2D axisymmetric mesh (580,000 elements)



- Elements are 0.1×0.1 μm
- Fixed time step, 4×10^{-10} s
- Ignition occurs ~10μm from electric match
- Al melt in front of wave
- Solidification of AlPt should occur at 1830 K



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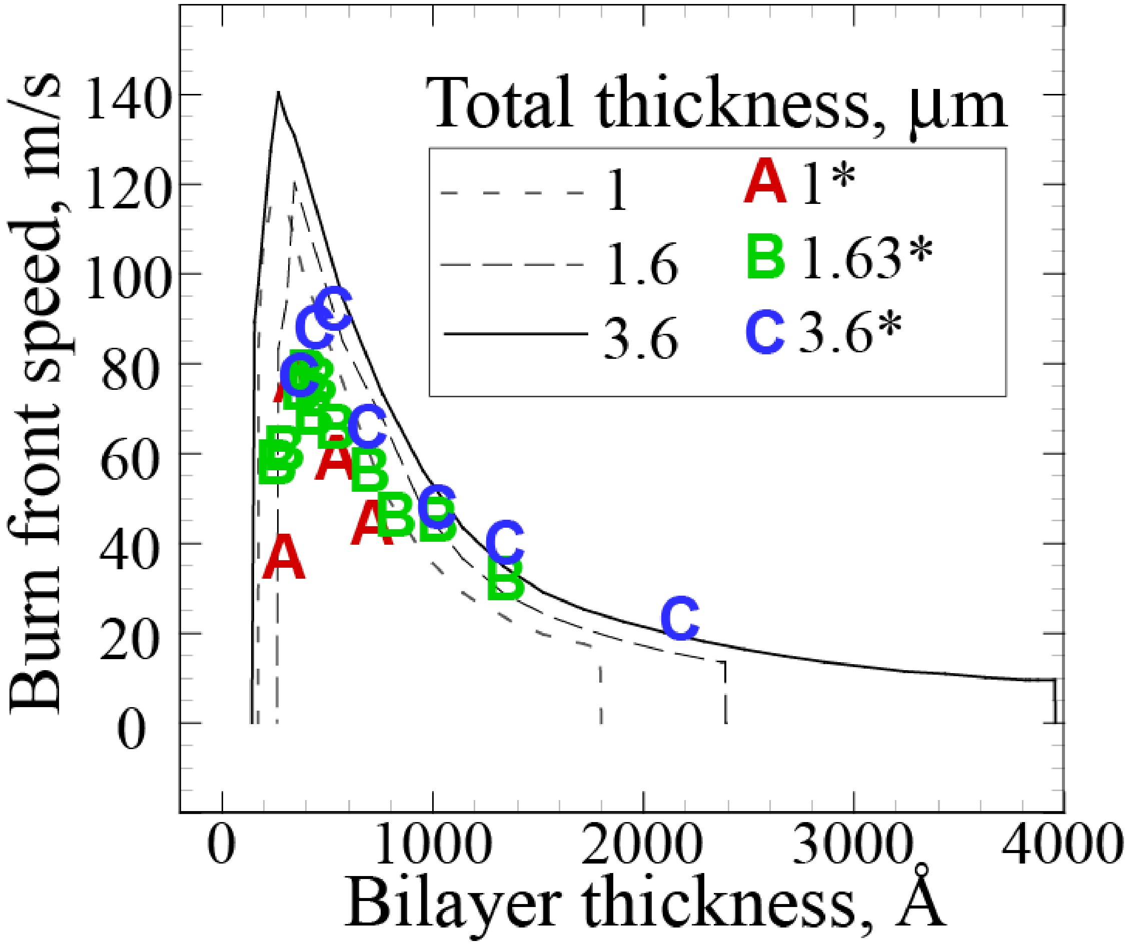
Front Velocity Variations with Bilayer Thickness



*Adams DP, Rodriquez MA, Tigges CP, and Kotula PG, “Self-propagating, high-temperature combustion synthesis of rhombohedral AlPt thin films,” *J. Mater. Res.*, Vol. **21**(12), pp. 3168-3179 (2006).

Summary and Conclusions

- The diffusion-limited model of Hardt and Phung has been used with a simple phase-change model to simulate the self-sustained, high temperature front propagation of Al/Pt nanolaminates on silicon substrates using a 2D axisymmetric finite element code.
- Results were within experimental uncertainty for nanolaminate thicknesses ranging from 1 to 3.6 μm
- Despite success, deficiencies should be addressed
  - Temperature dependent thermophysical properties
  - Solidification of mixed material
  - Strain due to thermal expansion
  - Adaptive mesh refinement
  - Stiff numerics

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