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REACTIVE NANO-FILMS OF AL AND PT

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Reaction front propagation rates of exothermic Al/Pt multilayer thin films sputter-deposited onto oxidized silicon substrates have been determined using a diffusion limited reaction model [1] along with the finite element code Calore [2]. Reaction front speed variations with total film thickness and bilayer thickness are similar to those measured by Adams et al. [3]. The front speed depends on ~100 Å-thick premixed interfacial layers, the amount of Al and Pt available for reaction, and the rate of diffusion. Fronts fail to propagate when bilayer thickness is less than a few hundred angstroms regardless of the total film thickness due to the premixed reactants. Front speeds increase when the bilayer thickness is between a few hundred angstroms and about 500 Å as a result of more Al and Pt available for reaction. Front speeds decrease as bilayer thicknesses increase above 500 Å as diffusive resistance increases. Eventually, the front ceases to propagate when the diffusive resistance is too great.

Figure 1.A shows a cross section of an Al/Pt multilayer film used for research of advanced joining technology (involving die attach and electronic packaging). Films were deposited within an ultra-high vacuum apparatus using direct current sputtering [3]. Figure 1.B shows a single ~100 Å-thick Al_xPt_y premixed layer between Al and Pt prior to combustion. The substrate used for these studies was oxidized silicon as shown in Fig. 1.C. The oxidized layer is about 4,000 Å thick. Figure 1.D shows a top view of the film at various times after ignition. An electric match was used as the igniter. The unreacted films are lighter in color than the reacted films.

A) Film cross section B) Bilayer interface C) Substrate X-section D) Top view

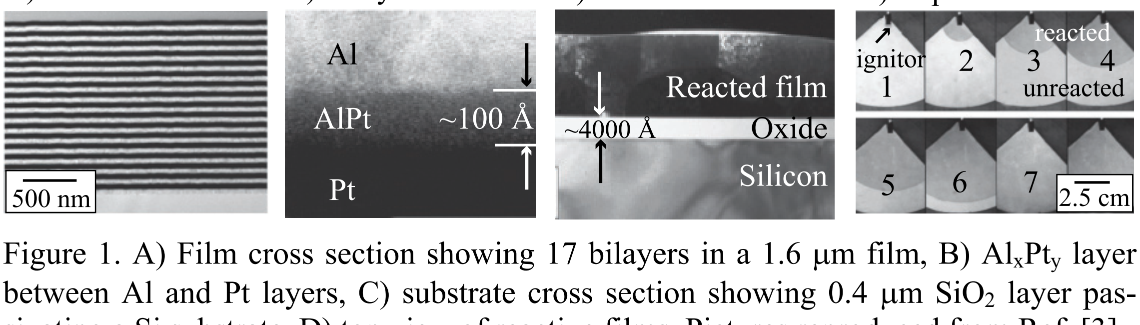

Figure 1. A) Film cross section showing 17 bilayers in a 1.6 μm film, B) Al_xPt_y layer between Al and Pt layers, C) substrate cross section showing 0.4 μm SiO_2 layer passivating a Si substrate, D) top view of reactive films. Pictures reproduced from Ref. [3].

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The reactive film is modeled as a continuum since the dimensions of the film are too small to represent discretely. For example, the ~100 Å Al_xPt_y layers would require 25 billion elements to model the system shown in Fig. 1.D with 3 elements thick, using a 2D axisymmetric geometry. Furthermore the time steps would be prohibitively small. The continuum assumption is used to model the reactive films with a constitutive model similar to Hardt and Phung [1]. Melting of the Al and Pt layers are modeled with an effective capacitance model. Radiative heat loss to the surroundings and conductive heat loss to the substrate are also considered. Typical bulk properties are used for Al, Pt, SiO_2, and Si. The properties for AlPt were determined from standard mixing rules (*e.g.* mass averaged specific heat, volume averaged conductivity, etc.).

Figure 2.A shows several 2D axisymmetric contour plots of temperature. The radial and axial dimensions are 200 and 29 μm, respectively. The thicknesses of the multilayer, SiO_2, and the Si substrate were 3.6 μm, 0.4 μm, and 25 μm, respectively. The bilayer thickness was 1907 Å. The 2D quadrilateral elements were 0.1 μm × 0.1 μm giving 290 elements in the axial direction and 2,000 elements in the radial direction for a total of 580,000 elements. Fixed time steps of 4×10^{-10} seconds were used for the calculations which ran on 32 dual core processors in about 2 hours. Figure 2B shows the reaction front speed as a function of bilayer thickness for three different total film thicknesses. The measured and calculated speeds show the same trends.

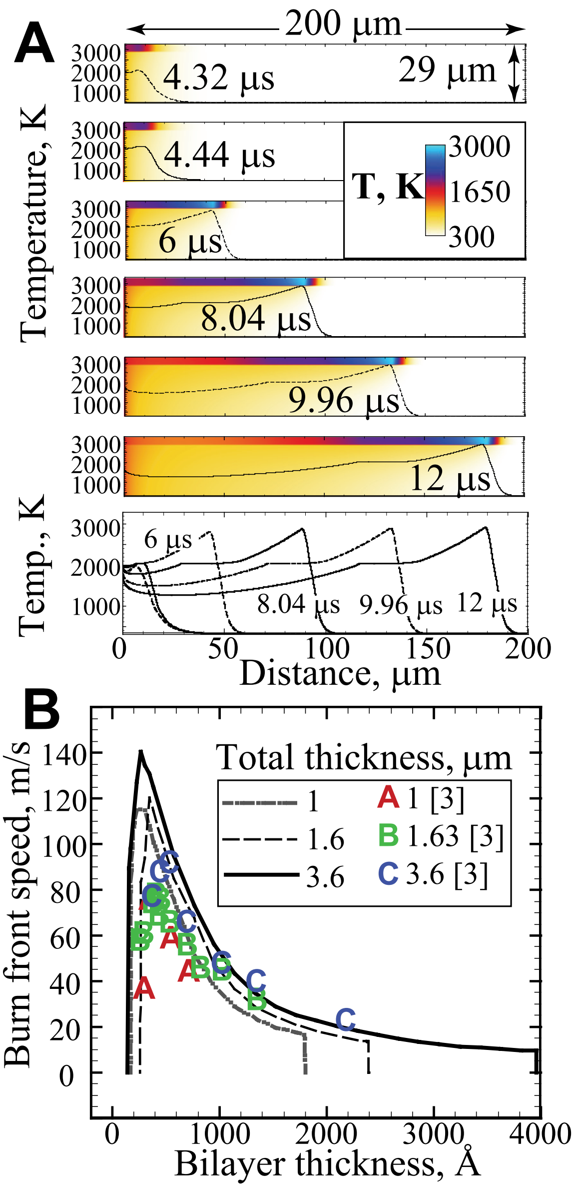

Figure 2. A) Temperature contour plots when bilayer is 1907 Å thick. Wave velocity is 22.4 m/s. B) Effect of bilayer thickness and total reactive film thickness on front speed. Lines are calculations and symbols are data from Ref. [3]

REFERENCES

[1] A.P. Hardt and P.V. Phung, "Propagation of Gasless Reactions in Solids—I. Analytical Study of Exothermic Intermetallic Reaction Rates," *Comb. and Flame*, Vol. **21**, pp. 77-89 (1973).

[2] S.W. Bova, K.D. Copps, C.K. Newman, *Calore—A Computational Heat Transfer Program*, Sandia National Laboratories Report SAND2006-6083P, Albuquerque, NM, 2006.

[3] D.P. Adams, M.A. Rodriguez, C.P. Tigges, and P.G. Kotula, "Self-propagating, high-temperature combustion synthesis of rhombohedral AlPt thin films," *J. Mater. Res.*, Vol. **21**(12), pp. 3168-3179 (2006).