

NUMERICAL SIMULATION OF REACTIVE MULTILAYER NANOFOIL HEAT TRANSFER

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Introduction

Nanostructured thin film materials have attracted a great deal of interest recently due to their unique mechanical, thermal, electrical and optical properties. A so-called nanofoil[®] has alternate layers of two materials, which can be easily fabricated using sputtering deposition^[1] or electron beam evaporation^[2]. The overall thickness of a typical reactive nanofoil is in the order of 10–500 μm, and the multilayer period is in the order of nanometers. One potential application of reactive nanofoils is to use the reactive foils as a controllable, localized heating source for joining applications, which will enable soldering and brazing of materials at room temperature.

In this paper, the authors present the multiphysics-based numerical simulations of reactive nanofoil Al/Ni multilayer system heat and mass transfer using COMSOL^[3]. The conductive heat transfer and mass diffusion equations are solved for 1D, 2D and 3D cases. With a small thermal pulse, atoms diffuse into the companion layers, and Al-Al and Ni-Ni bonds are exchanged for Al-Ni bonds. This local bond exchange produces a large quantity of heat that is conducted down the foil and facilitates more atomic mixing and compound formation, thus establishing a self-propagating reaction.

Numerical Modeling

A reactive nanofoil of 0.6 m in length was simulated. The chemical composition variation due to reaction can be modeled using the diffusion equation.

$$\partial C / \partial t + \nabla \cdot (-D \nabla C) = R \quad (1)$$

Where R is the reaction rate (reaction constant times chemical composition C , when $T > 500^\circ\text{K}$, was used in the simulation); and D is the diffusion coefficient in m^2s^{-1} . The values $E = 137 \text{ kJ/mol}$ and $A = 2.18\text{E-}6 \text{ m/s}^2$ were used in the present study following Jayaraman et al.^[4]. The heat conduction equation is used to simulate the temperature field in the reactive nanofoil. The heat conduction equation and the mass diffusion equation are coupled together

using the local temperature and concentration, as shown below.

$$\rho \times c_p \times \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = \dot{Q} \quad (2)$$

where C_p denotes the specific heat capacity, T is temperature, k is the thermal conductivity, ρ is the density, and \dot{Q} is related to the changing rate of the nanofoil composition.

Numerical Simulation Results

Figure 1 shows the flame speed variation as a function of the reaction constant.

Armstrong and Koszykowski^[5] presented an analytical solution for bi-layered nanofoils with an ideal composition profile. They found that the flame speed was proportional to $1/\delta$, where δ was the foil bi-layer thickness. The flame speed also depends strongly on the maximum reaction temperature. As reported by Gavens et al.^[6], for a nanofoil with 200 nm bi-layer thickness, the flame speed was in the order of 1 m/s. This speed corresponds to the reaction constant of 3000 in our simulation. For a thin bi-layer thickness of 30 nm, a flame speed of 10 m/s could be achieved, which would correspond to a reaction constant approximately 60,000.

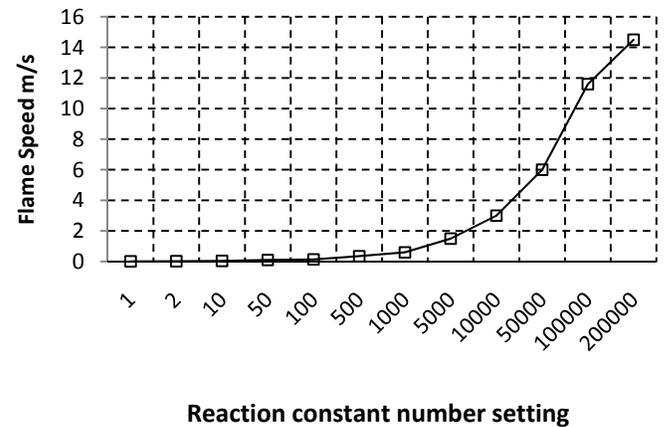


Fig. 1 The flame speed versus the reaction rate

For the 2D case, the calculation domain includes a layer of Al and a layer of Ni, and two mass diffusion equations are used. The Al/Ni bi-layer is assumed to have a perfect interface initially, with no heat loss being considered in the simulation. As it takes both Al/Ni to trigger the reaction, the temperature change starts from the Al/Ni interface, Fig. 2.

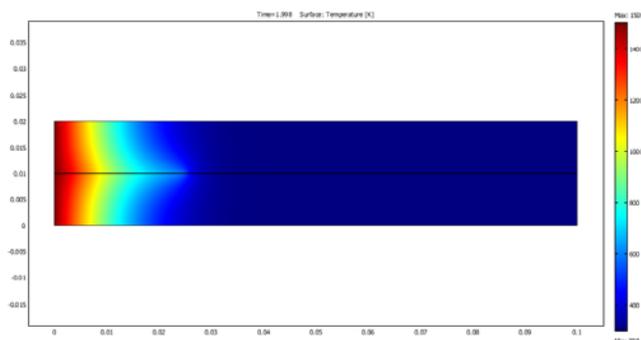


Fig. 2 The 2D case: temperature distribution in the Al/Ni bi-layer.

In the 3D simulation, reactive nanofoils are applied onto a substrate block of silicon. A flame speed of 5 m/s is prescribed with a heat flux density of $1.5 \times 10^8 \text{ W/m}^2$, which represents the heating value of a nanofoil tested by the authors. Temperature histories at two locations are presented in Fig.3. PT1 is 100 μm underneath the foil/wafer interface along the middle line of the nanofoil; and PT2 is 100 μm away from the edge of the nanofoil but on the top surface of silicon wafer. These two points are selected to monitor the temperature distributions during the reactive joining process. The flame front hits PT1 at time=18 ms, Fig.3. Although the surface of nanofoil has a maximum temperature above 1000°K, the substrate has a very moderate temperature change. At the location of PT1, it peaks at about 465°K in the simulation. The heat is absorbed quickly by the silicon substrate and the temperature drops due to the heat conduction in silicon wafer and the natural convection to the ambient surrounding. Half second after the passing of the flame front, temperature decreases to 360 °K at PT1. At the location of PT2, 100 μm away from the edge of the nanofoil on the surface of silicon wafer, the maximum temperature is found to be 402°K. Within 0.5 second, the temperature drops to 360 °K. From the simulation, it is evident that when using reactive nanofoils for microchip bonding, the heating affected region is localized. A short distance away from the heating foil, the maximum temperature is less than 500 °K and the wafer temperature decreases to a low bulk temperature in less than one second.

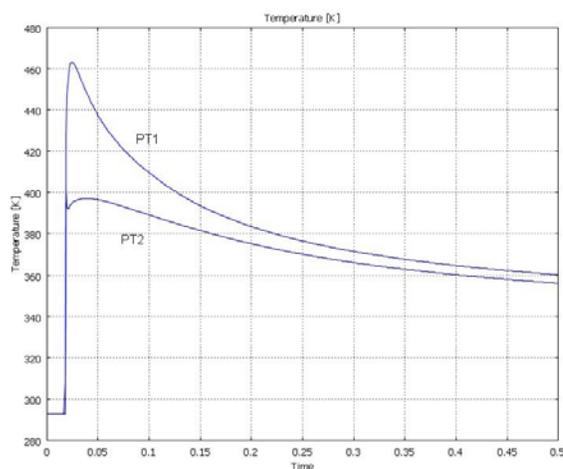


Fig. 3 Temperature increase on the silicon wafer

4. Conclusions

Performance of reactive nanofoils is studied under 1D, 2D and 3D configurations using multiphysics based numerical simulations. The flame speed is successfully modeled as a function of the chemical reaction rate. The detailed chemical compositions have been obtained for the Al/Ni bi-layer foil. The performance of nanofoil is quantified in terms of temperature and species distributions, and the flame speed. The numerical simulation proves that the heating from a reactive nanofoil to the substrate is highly limited and localized.

Acknowledgments

R.R.Liu is supported by a LSU EDA scholarship.

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