Numerical Investigation on the Oscillatory Propagation of Intermetallic Reaction Waves in Microscale Aluminum/Nickel Multilayers

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1 Introduction

The novel concept of microscale reactive multilayer foils features high possibility of performance improvement in many advanced applications including micron-sized pyrotechnic initiation system for explosives/propellants ignition and high precision joining or bonding in micro-device manufacturing processes [1-3]. The reactive multilayers are generally comprised of two alternating metallic layers of nanometric thickness and could be efficiently manufactured by metallic vapor deposition of magnetron sputtering or electron beam evaporation as well as the mechanical pressing of stacked metallic foils. When ignited by the external heat source, the reactive multilayer foils show various desirable pyrotechnical features such as highly tunable ignition delay and self-sustained intermetallic reaction wave propagation. The reaction wave speed could reach tens of kilometers per second, as demonstrated by several experimental studies, and the tests also show a very short ignition delay [4].

So far, there exist various numerical modeling studies to investigate the self-propagating reaction waves in bimetallic multilayers by utilizing the transient intermetallic diffusion or reaction models and also quasi-steady approximation model [5-8]. In present numerical investigation, the intermetallic reaction wave propagations in reactive bimetallic multilayers are studied to capture and better understand the oscillatory behaviors of self-sustained reaction wave propagation.

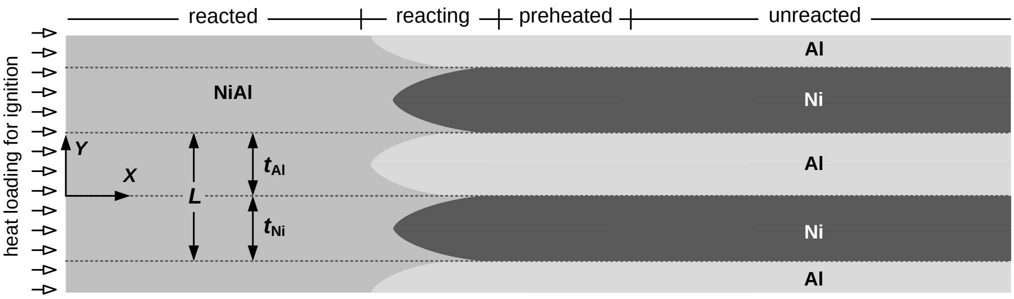

Figure 1: Schematic on the intermetallic reaction wave propagation in microscale Al/Ni multilayers.

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2 Numerical Modeling of Reaction Wave Propagation

The numerical model features the simple geometry of alternatively stacked thin foils of many nanoscale aluminum/nickel (Al/Ni) bilayers, as illustrated in Fig. 1. The governing equations are consisted of time-dependent two-dimensional Al/Ni atomic species diffusion and thermal diffusion for the simulation of self-propagating reaction waves. The intermetallic reaction from Al and Ni layers to NiAl is here assumed to obey diffusion limited reaction kinetics and the binary atomic diffusion coefficient is based on Arrhenius dependence with temperature [5-7]. The reaction ignition was realized by imposing the heat flux on the left side for a pre-determined time period which simulates the experimental method of laser or hot-wire ignition. Detailed description of numerical model and computational method could be found in the previous numerical study [8].

Continuing and present studies have been investigating the effects of various geometric parameters. The numerical results shown here are for bilayer spacing of L = 20 nm with stoichiometric layer thickness ratio of t_{Al}:t_{Ni} = 3:2. The necessary existence of atomic premixing at the Al/Ni interface is also included in the numerical model. The numerical results for the model validation in Fig. 1(a) present the effects of bilayer spacing on the reaction wave speed with premixing thickness of 1.2 nm. Fig. 1(b) shows the effects of premixing thickness on the reaction wave speed with bilayer thickness of 20 nm. The prediction results of reaction wave speed in both figures give good agreement with corresponding ignition test measurements of Al/Ni multilayer system [4].

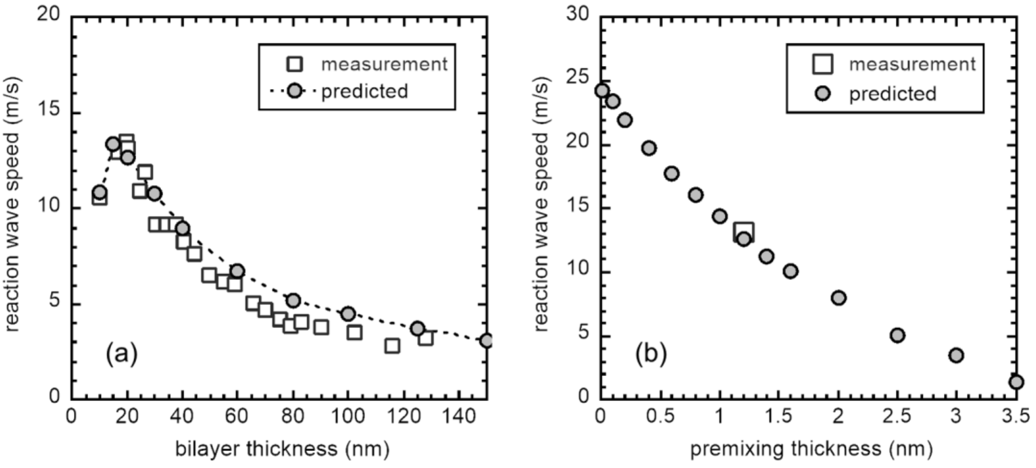

Figure 2: Model validation on intermetallic reaction wave propagation with the measurements. The effects of (a) bilayer thickness and (b) premixing thickness on time-averaged reaction wave speed in reacting Al/Ni multilayers. The measurement data are from Knepper et al. [4].

Fig. 3 represents the temporal evolution for spatial distributions of dimensionless atomic species concentration and reaction heat generation as well as temperature with the time interval of 50 ns. The results clearly show the advancing reaction waves after the occurrence of reaction ignition. Also, the oscillatory and periodic occurrence of reaction heat generation and subsequent fluctuation in temperature can be observed. This oscillatory behavior does not show up in case of no interface premixing. The time-averaged reaction wave speed is evaluated to be 12.9 m/s and it is in excellent agreement with measured speed of approximately 13 m/s.

In order to closely appreciate the effects of atomic premixing at the Al/Ni interfaces on oscillatory propagation of reaction waves, premixing thickness now increases to 2.4 and 3.0 nm, respectively, and the corresponding numerical results are shown in Fig. 4 by means of time-space contours for temperature distribution along the horizontal Al/Ni interface line. As expected, an increased degree of atomic premixing slows down the reaction wave propagation and also significantly amplifies the oscillatory behaviors of reaction wave propagation. As more clearly observed in the case for premixing thickness of 3.0 nm, the oscillatory characteristics in reacting Al/Ni multilayers show the sudden burst of reaction and periodic hot spots in high speed advancing of reaction waves followed by relatively calmed time period of much reduced reaction wave speed behind the reaction wave front in a periodic manner.

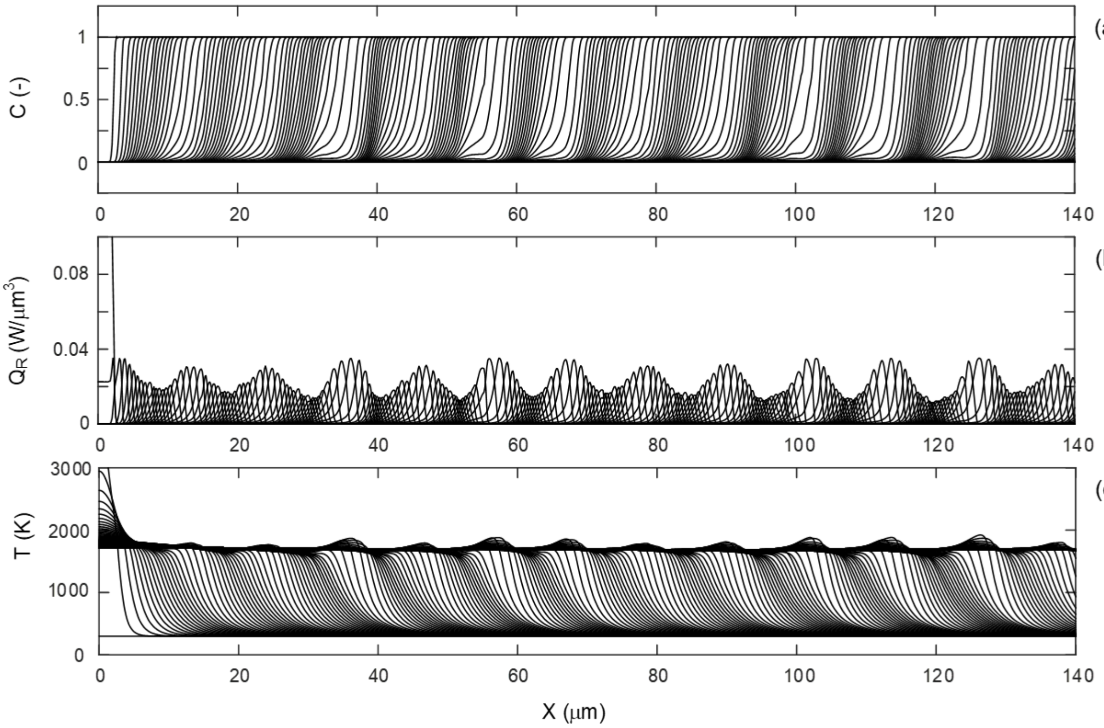

Figure 3: Transient progress of (a) Al species concentration, (b) reaction heat generation rate, and (c) spatial temperature in reacting Al/Ni multilayers with bilayer thickness of 20 nm and premixing thickness of 1.2 nm.

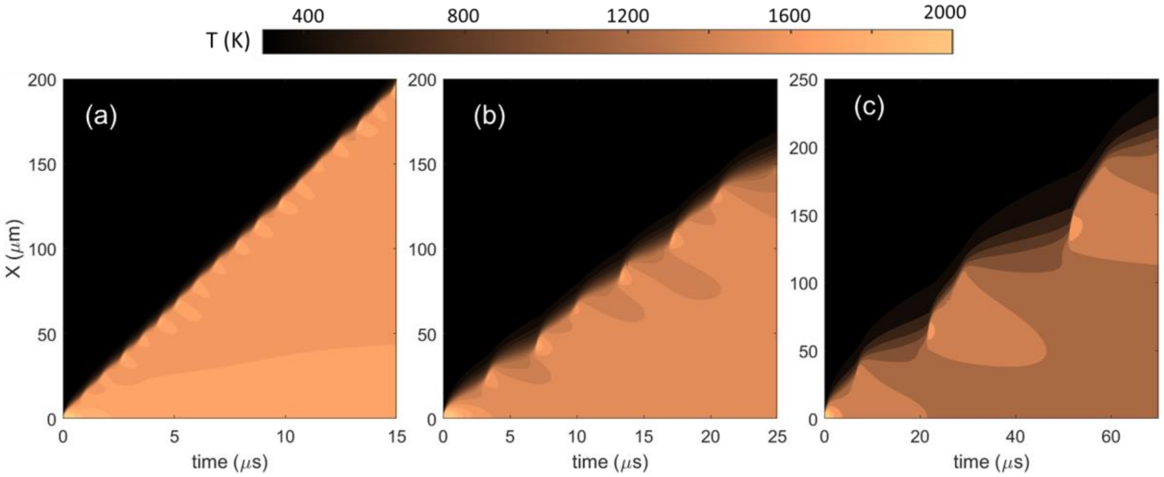

Figure 4: Time-space contours of temperature on the Al/Ni bilayer interface with premixing thickness of (a) 1.2, (b) 2.4, and (c) 3.0 nm. In all cases, bilayer thickness is 20 nm.

3 Conclusions

Present numerical model on the self-sustaining reaction wave propagation in microscale multilayers of binary metallic combination is well validated with measured reaction wave speed of Al/Ni multilayer ignition tests. If the conditions are met, the oscillatory behaviors of reaction wave propagation may occur in such reactive systems and, here in this study, it is found that the atomic premixing at bimetallic interface significantly promotes such an oscillatory unsteadiness and the complex characteristics of bimetallic reaction waves including periodic reaction bursts and hot spots.

Acknowledgments

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