Heat and Mass transfer in Reactive Multilayer Systems

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Introduction: Established joining techniques are characterized by a large amount of heat load of the components. Reactive multilayer systems (RMS) consist of thousand of alternating periodical layers of reactive materials, e. g. Al-Ni [3]. After a suitable ignition these layers can react exothermically with each other and melt a solder material.

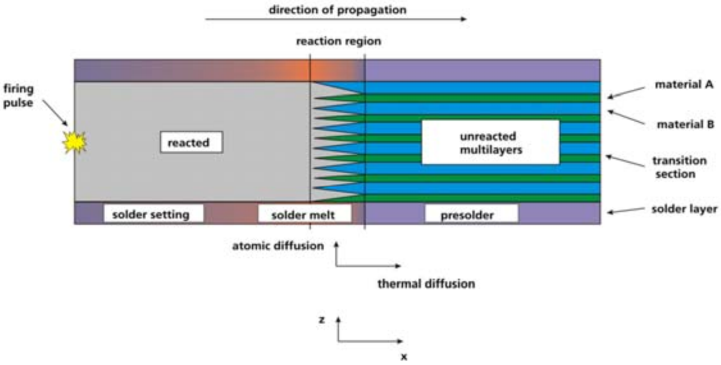

Figure 1. Principle of the reaction in the reactive multilayer systems (RMS).

Computational Methods: Atomic diffusion can be described by using a time-dependent scalar field *C(x,z,t)* [mol/m³] in the diffusion equation:

$$\frac{dC(x,z,t)}{dt} - D\cdot\frac{\partial^2 C(x,z,t)}{\partial z^2} = 0.$$

For the atomic diffusivity *D* the Arrhenius equation was assumed. The atomic diffusion releases a thermal wave in x-direction. This wave can be described by the heat equation:

$$\rho_i(T)\cdot c_{p,i}\cdot\frac{\partial T(x,z,t)}{\partial t} - k_i(T)\frac{\partial^2 T(x,z,t)}{\partial x^2} = Q(C).$$

For the concentration dependent heat source *Q(C)* [W/m³] the following ansatz from [1] has been used:

$$Q = \frac{H\cdot M^2}{\rho(T)}\cdot\left(\frac{\partial C(x,z,t)^2}{\partial t} + v_{Diff}\cdot\frac{\partial C(x,z,t)^2}{\partial x}\right).$$

Results: The temperature profiles *T(x,z,t)* of RMS with different period thicknesses between 50 nm and 100 nm have been calculated with the same Al to Ni atomic ratio (figure 2). Furthermore the influence of different atomic ratios N_{Al}/N_{Ni} has been modeled from 40 at-% to 55 at-% Al in the period (figure 3). The calculated velocities of the thermal front v_{calc} have been compared with experimental measured velocities v_{exp} (figure 4).

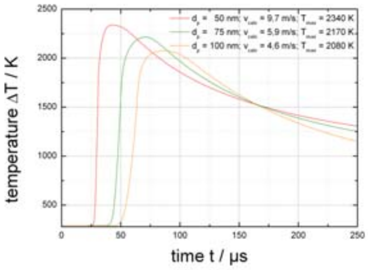

Figure 2. *T* as a function of the periodic thickness d_p.

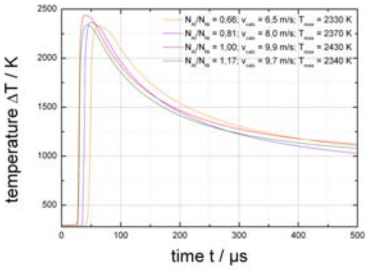

Figure 3. *T* as a function of Al/Ni atomic-ratio.

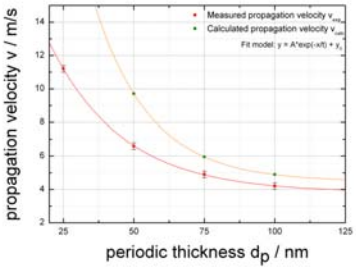

Figure 4. Velocity *v* as function of the periodic thickness d_p; calculated and experiment velocity *v*.

Conclusions: We have simulated the temperature, the velocity and the melting time of the RMS. Based on the simulation a multilayer design can be fabricated for specific application. Based on these findings it is possible to produce RMS for the industry.

References:

1. R. Armstrong, Theoretical models for the combustion of alloyable materials, *Metallurgical and Materials Transactions A*, **Vol. 23**, 2339 No.9 (1992)
2. A.B. Mann, A.J. Gavens, M.E. Reiss, D. Van Heerden, G. Bao, T.P. Wheis, Modeling and characterizing the propagation velocity of exothermic reactions in multilayer foils, J. Appl. Phys., **Vol. 82**, 1178 (1997)
3. G. Dietrich, M. Rühl, S. Braun, A. Leson, Hochpräzise Fügungen mittels reaktiven Nanometermultischichten, Vakuum in Forschung und Praxis, **Vol. 24**, 9 No.1 (2012)

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