REGIMES OF SYNTHESIS IN THE NANOSCALE MULTI-LAYER Ni/Al FILMS ON A SUBSTRATE

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Synthesis of nanoscale intermetallic, oxide and nitride films is a new technological method for production of coatings with unique properties for a variety of practical applications. The Ni/Al system is one of the most widely studied. Because of a high melting temperature (1638 ^{o}C) of NiAl and its high chemical stability, the films of this material can be used as protective coatings for various machine components. A new and rapidly expanding area of research and development is the application of Self-Propagating High-Temperature Synthesis (SHS) in thin metal-metal films (including the Ni/Al system) for joining (soldering or welding) of temperature-sensitive and small-sized components [1,2]. Raw nanoscale layers have high reactivity due to a very short interdiffusion time. Because of this, carrying out the synthesis reaction in the regimes of combustion wave propagation or thermal explosion permits performing joining during a very short time (~ 10^{-1} -10^{-2} c) and with small specific heat release (heating of the system as a whole does not exceed 10-20 ^{o}C). The latter is especially important for joining such temperature-sensitive materials as metallic glasses. Local heating during SHS in nanofilms also permits joining materials with substantially different coefficients of thermal expansion, for example, joining a metal to ceramics.

Despite a large number of the studies on the thermodynamics, kinetics and dynamics of SHS in Ni/Al nanofilms there are two problems related to this process that have not been solved in a sufficiently accurate way till now. The first problem is a detailed examination of the effect of heat losses into the substrate and the second one is a rigorous investigation of the growth of different-phase layers taking into account both the diffusion processes and the realistic phase diagram of the system. The latter problem is treated in full in the paper by B.B. Khina presented in these proceedings [3]. The former problem is analyzed in this work and is aimed at two-dimensional modeling of two conjugate processes: propagation of the synthesis wave in the multi-layer Ni/Al system and propagation of the thermal wave into the substrate. The main question addressed in this work is the following: what are the conditions (first of all, the number of Ni/Al binary layers, initial temperature and heating rate) for the development of self-sustaining reaction towards complete formation of the final product.

The geometry of the computational region and boundary conditions are presented in Fig. 1.

The basic assumptions of the developed mathematical model are the following:
– the film is isothermal in the transverse direction;
– the thermal contact between the film and the substrate is ideal, i.e., the temperatures and heat fluxes at the interface y=h are equal;
– the growth of the product layer is determined by simplified diffusion kinetics (quasi-steady-state approximation);
– the thermophysical properties of the system are constant.

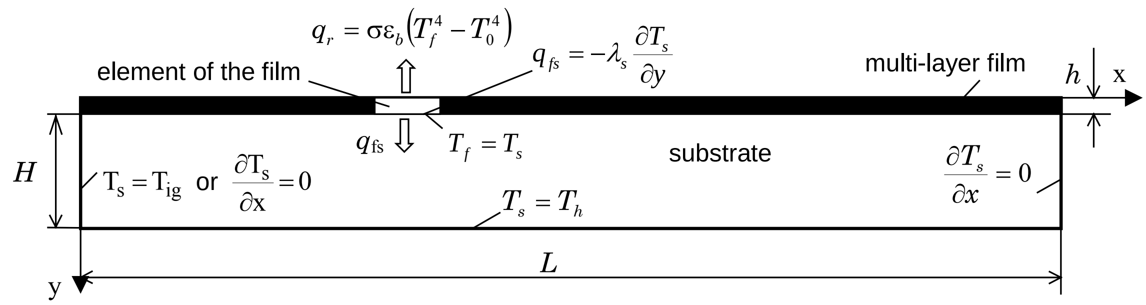

Fig. 1. Sketch of computational region and boundary conditions for the energy transfer equations

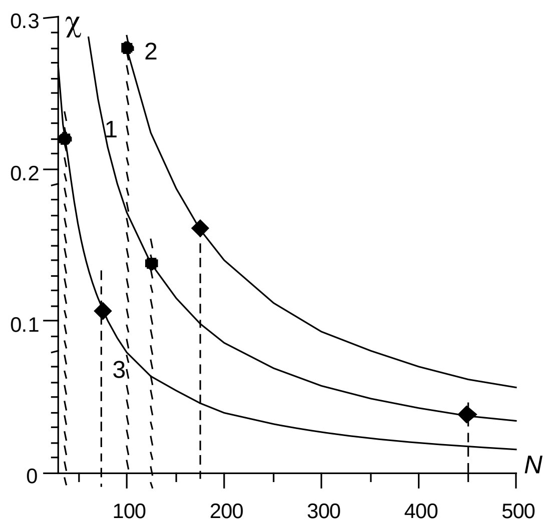

Fig. 2. Parameter χ vs. the amount of binary layers in a Ni/Al film on a glass substrate. Numbers at curves correspond to different values of the interdiffusion coefficient: 1, Ref.[4]; 2, Ref.[5]; 3, Ref.[6]. Rhombs denote the limits of SHS for initial temperature 300 °C and circles for 450 °C

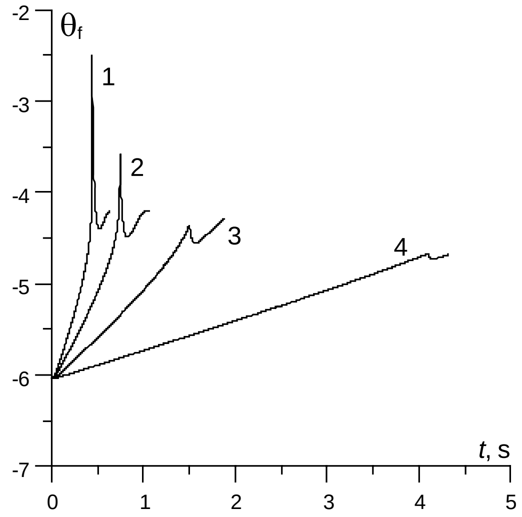

Fig. 3. The film temperature vs. time for different heating rates in the thermal explosion regime for χ=0.1 (75 binary layers with the interdiffusion coefficient taken from Ref. [6]). The heating rates are 339 K/s (curve 1), 203 K/s (2), 102 K/s (3) and 33.9 K/s (4)

Synthesis in multi-layer nanofilms can be performed in three substantially different regimes: (i) the regime of self-sustaining propagation of a combustion wave, (ii) the thermal explosion regime and (iii) the annealing regime. The analysis of the governing equations describing the synthesis process shows that the most important dimensionless parameter defining the limits for the regions of different regimes is $\chi = \left(\sqrt{a_s/8D_*}/N\right)\left(\rho_s c_s/\rho_f c_f\right)$, where a_s is the thermal diffusivity of a substrate, D_* is the interdiffusion coefficient, N is the number of binary layers, $\rho_i c_i$ is the thermal effectiveness of the film ($i \equiv f$) and substrate ($i \equiv s$). It is noteworthy that the parameter χ is determined only by the amount of binary layers N but does not depend on the binary layer thickness. This amount should be rather large for the regime of self-propagating wave, tens or even hundreds binary layers. For lower N the SHS regime is impossible. The critical numbers of binary layers for the Ni/Al system are obtained by numerical modeling and are plotted in Fig. 2. Modeling has also demonstrated that SHS in the films deposited on metallic substrates is substantially more hampered in comparison with glass substrates.

For synthesis in the regime of thermal explosion to be carried out, along with having a large number of binary layers, it is necessary to perform fast uniform heating of the film and substrate. Figure 3 illustrates the dynamics of the film temperature for thermal explosion at different heating rates.

Acknowledgements

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