

MODELLING INTERACTION KINETICS DURING SHS IN THIN-FILM NI-AL SYSTEM: A DIAGRAM OF PHASE FORMATION MECHANISMS

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Self-propagating high-temperature synthesis (SHS) in a multilayer thin-film (10-1000 nm) and thick-film (10-100 μm) Ni-Al system is used for producing oxidation-resistant NiAl coatings on Ni-base superalloys, joining a NiAl layer to bulk alloys, welding of amorphous alloys to bulk crystalline materials, welding of microobjects (microwelding), etc. [1]. Despite a large number of experimental works [1-4 and many other], the phase and structure formation mechanism during SHS in this system is not well understood. According to Ref. [2], interaction of liquid Al with solid Ni during SHS in powder mixtures occurs “through a continuous forming and dissolving of a reaction diffusion layer on the surface on the Ni particle”, which corresponds to the equilibrium Ni-Al phase diagram. On the contrary, in Ref. [3] it is concluded that at $T > T_m(\text{NiAl}_3) = 1127 \text{ K}$ “the system consists of only solid nickel and liquid aluminum solution”, i.e. structure formation has a substantially non-equilibrium nature and occurs via dissolution of Ni in molten Al and precipitation of NiAl grains from supersaturated melt, which agrees with the experimental results obtained on thick foils [4]. In the films, SHS may proceed via a solid-state diffusion-controlled growth of the product layer, NiAl. This concept was used in modeling SHS in this system, but the parameter values (activation energy E and preexponent D_0) were determined by the data fitting to obtain a match between the calculated and experimental data [5]. In this case, these parameters lose their physical meaning: they describe SHS as a whole but not a particular underlying physico-chemical process. In our recent work [6] on the basis of the realistic parameter values (diffusion characteristics of the product phase and experimental temperature profile of an SHS wave) it has been proved that during SHS of interstitial compounds such as carbides, nitrides, etc. in the wave propagation mode only the non-equilibrium dissolution-precipitation mechanism of the final product formation can take place.

In this work, a rigorous mathematical model for SHS in a layered Ni-Al system is developed, relying on the “solid-state diffusion-controlled growth” approach for a substantially non-isothermal situation. Two competing processes are considered: (i) growth of NiAl layer between solid Ni and liquid Al due to solid-state interdiffusion in this phase (a quasi-isothermal submodel), and (ii) dissolution of NiAl in both liquid Al and solid Ni because of the inclination of solidus and liquidus lines of the Ni-Al phase diagram (a non-isothermal submodel). Thus, the thickness of the solid product phase (NiAl) obtained at the attainment of the adiabatic SHS temperature is determined by competition of the above two “elementary” processes. In the mathematical formulation of the model, a difference in the densities of all the phases is considered, and the density of nickel-containing Al melt is determined taking into account its temperature dependence [7]. For computer simulation, spline-approximation of solidus and liquidus lines of the Ni-Al phase diagram is used. Diffusion parameters for the growing phase, E and D_0 , are taken from the independent experimental works on solid-state diffusion in NiAl [8,9]. Modelling is performed for different heating rates. The examined situation corresponds to SHS in the thermal explosion mode.

As a final result of modeling, a diagram of phase and structure formation mechanisms during SHS in this system is built. At high heating rates and sufficiently thick layers of reacting metals (Ni and Al), the solid-state diffusion-controlled mechanism of the NiAl layer growth is impossible because the thickness of the solid NiAl interlayer falls down to zero, and thus in a certain parametric range only the non-equilibrium dissolution-precipitation mechanism can operate. For thin films, the quasi-equilibrium “solid-state diffusion-controlled growth” mechanism can work even at high heating rates typical of SHS in the wave propagation mode, $dT/dt \sim 10^6 \text{ K/s}$.

References

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