

Mesh-Free Modeling and Control of Thermal/Diffusion Fields Created by Nanosources

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I. ABSTRACT

Since the early days of mankind, thermal processing of materials has played a pivotal role in the advancement of human civilization. Today, thermal processing is still found to be at the heart of the modern manufacturing industry, playing a primary role in surface engineering, microelectronics, chemical/biomedical technologies etc. Despite the numerous scientific and engineering accomplishments in macro- and microscale thermal processing, however, the on-going technological advancements in nanoscale science and engineering, as well as the constantly growing demand for miniaturization of engineering components and devices have presented unprecedented challenges to the currently existing thermal manufacturing technologies and theory.

To this end, in this paper we present an analytical model of the temperature and concentration dynamic distributions generated in a substrate material from the exothermic material transformations of nano-thick reactive thin films (such as nickel and aluminum) deposited on the substrate's external surface. Successful modeling and in-process regulation of the energy generation from such nano-sources is of primary importance in several industrial applications, such as rapid thermal processing of semiconductor wafers, micro-electro-mechanical systems packaging etc. The model, which is computationally parallel and meshless (i.e., decoupled with the capability to be solved numerically in real time) is based on a system of lumped energy and mass balances, currently existing kinetic growth theories, and Green's function analysis. Green's functions have been used extensively in macro- and microscale modeling and are currently attracting much attention for use in nanoscale applications (non-equilibrium Green's functions). The developed model is validated with nickel aluminide coatings of micrometer thickness processed on a robotic plasma arc laboratory station, through in-process infrared thermal sensing and off-line metallographic analysis.

Finally, an analytical Green-Galerkin method is also presented which allows to 1) computationally identify the internal temperature field that is achieved within the volume of a three-dimensional solid by surface temperature measurements alone (obtained by thermocouples and/or infrared pyrometry), and 2) control the three-dimensional temperature field that is generated inside the volume through external surface heating (applied by the nano-sources).