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A Simulation Approach to the Combustion Synthesis of Silicides

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ABSTRACT

The work describes the application of a computer simulation approach developed by the authors to the study of the SHS of some disilicides $MeSi_2$ (Me = Mo, Nb, Ta, Ti).

The method is specifically oriented towards the study of the reaction mechanism and of the heterogeneous aspects of the SHS process and takes into account solid/liquid phase transitions, diffusion-controlled dissolution of the high melting metal and nucleation/precipitation of the compound. When combined with experimental measurements, the computer approach is able to outline the effect of the various process variables, to obtain a microscopical insight of the reaction mechanism and to determine the onset of different dynamic behaviors.

The reported results are compared with experimental literature data with particular attention to the effect of starting reactant grain size and of the effective thermal conductivity of the powder mixture.

Keywords*:* SHS, simulation, disilicides.