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A Computational Model for the Si/C/N Nanopowder

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The growing interest in the synthesis of Si/C/N nano-sized powders can be further highlighted by the fabrication of materials that offer a large scale of properties. The powder must have a high purity and specific morphological characteristics depending strongly on the employed experimental process. Several methods are employed to produce ceramic powders from vapour phase reactants. These include flows through a tube furnace, Rf-heated and plasma arc. The presence of hot walls in these methods is undesirable since they can act as heterogeneous nucleation sites and sources of unwanted contamination. Furthermore, the thermal profiles within the reaction zone of these methods are often complex and give rise to non-uniform nucleation and growth, inducing irregular characteristics. To overcome this problem a new method was recently developed in the Massachusette Institute of Technology. An infrared CO2 laser beam is used to heat gas by absorption of radiation. The principle reason for this is due to the small size of the reaction zone minimizing the contamination area. In this work laser-heated gas-phase synthesis process is considered. The laser beam and gas stream interacts in orthogonal direction (cross flow). The precursor gas is continuously injected into a reaction chamber, which after reaching a threshold temperature of approximately 600°C reacts and decomposes thermally. The central inner jet is bounded by a coflowing annular inert gas (argon). It is interesting to note that the laser energy is not directly used to heat the argon gas. This is due to the fact that argon does note absorb the line emitted by the laser. The aim of this investigation is to develop an improved fundamental understanding of the heat and mass transfer during the synthesis of nanopowder ceramics. One aspect of this understanding consists to, determine 3D distribution of temperature and species, coupled to the fluid flow in the reactor. A numerical model is developed and simulations are conducted by using CFX5 CFD software based on finite volume approximation. It was also hoped that this study would allow a better understanding for the particles formation, in order to achieve the ultimate goals of an ideal powder synthesis.

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