On the Stability of High-Performance Crystal Growth Simulations by the MPFC Method

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Abstract: Computer modeling of crystal growth processes is often associated with complex numerical calculations. The results of such calculations cannot always be predicted. In some cases, the features of mathematical methods of calculation in conjunction with the assumptions of mathematical models can lead to the appearance of unexpected results. Such results on the one hand will be correct from a mathematical point of view, but on the other hand they will not have physical justification and experimental confirmation. Obviously, in such cases it is necessary to carefully process the results obtained taking into account the physical meaning and to avoid false conclusions. And it is especially important to take this into account in the case of large-scale high-performance simulations. Earlier, high-perfomance computational algorithm for the modified phase field crystal model (MPFC) of crystal growth were formulated [1] and the results of some three-dimensional simulations are obtained [2]. In current paper we present some unstable results of simulations by the MPFC and discuss such a phenomenon.

Keywords: Mathematical modeling, simulations, crystal growth, phase field crystal

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