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COMPUTER-AIDED MODELING OF HIGH-PRESSURE/HIGH-TEMPERATURE PROCESSING OF MATERIALS

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ABSTRACT

Introduction. Modern industry and technology make wide use of technological processes, which feature an interrelation between electrical, temperature, mechanical and concentration fields. They are, first of all, the processes of heat treatment, phase transformations in straining and electric heating as well as mechano-chemical processes, etc. Among coupled processes are processes occurring in a solid-phase high pressure apparatus (HPA) in heating it and synthesizing (or sintering) superhard materials in it.

Theoretical model. Present paper deals with the numerical modeling of the diamond crystallization process in a HPA. This process is accompanied by the multi-physics processes of electric resistance heating, thermoelastoplastic deformation and graphite-to-diamond phase transitions. Thermodynamics and kinetics of diamond crystallization are greatly influenced by the coupling between fields of electric potential, temperature, pressure and various volume fractions in a reaction zone of HPA.

Two scale levels are considered: the whole HPA (first level) and the individual diamond crystal growing in the metal melt (second level). To describe the above process on the first level the numerical technique for FEM solving of coupled nonlinear nonsteady problem of electroheat conduction and thermoplasticity, taking into account the large elastoplastic strains, phase transitions of materials and high pressure effect, has been developed [1, 2]. All equations are written for effective values of physico-mechanical properties. Phase transitions are determined from the changes in properties, volume fractions and abrupt change in specific volume in the region where diamond synthesis is possible. The coupling of the above equations is caused by the following dependences: of physico-mechanical characteristics on pressure, temperature and volume fractions; of field of Joule heat sources on temperature; of volume fractions fields on temperature and stress distributions.

For the second level we take the following calculation scheme: a spherical diamond crystal surrounded by spherical layers of solvent-metal melt and graphite. The pressure and temperature at any point of reaction mixture determined from solving the problem for the first level is applied to outer surface of graphite. Then, the thermodynamic criterion of phase transition is entered, which takes into account inhomogeneity and

nonhydrostatic character of the stress-strain state in the diamond-melt-graphite system and describes the area of transformations. The closed connection of solutions of the mechanical tasks at two scale levels is installed by the coordination of elastic modules of a reaction mixture and local diamond-melt-graphite system.

Results. A problem on determination of temperature, stresses and volume fractions fields in the reaction zone of HPA and in the local diamond-melt-graphite system under diamond synthesis conditions has been solved. The results demonstrate: a significant coupling of these fields; an interrelation of the solutions for the reaction mixture and for the local diamond-melt-graphite system; the effect of self-regulation of pressure in the HPA reaction zone consisting in pressure oscillation with respect to graphite-diamond phase transition line.

To clarify the influence of phase transitions on thermostressed state of HPA, a similar problem has been solved but without regard to phase transitions. The solution of the problems considered supports the need for an obligatory allowing for the coupling of the processes and phase transitions when simulating physico-mechanical state of the HPA reaction zone.

The experimental and calculated results of diamond synthesis in various HPAs are considered depending on the volume of a reaction cell, thermodynamic parameters of the process, composition and the scheme of an arrangement of reaction charge components [3]. Comparison between calculated and experimental results has confirmed potentiality and expediency of the efficient use of computer-aided modeling for the development of new technologies of diamond synthesis.

The examples are given of the use of the developed numerical technique for calculation of crystallization zones of cubic boron nitride, modeling of temperature conditions in the reaction cell during crystallization of gallium nitride, determination of conditions of efficient sintering of cBN-based polycrystalline materials, modeling of thermostress state and optimization of parameters of thermobaric processing of high-temperature superconducting ceramics in a HPA [4] and so on.

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