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3-D Modeling of Particle Size Reduction from Micro to Nano Scale Using Finite Difference Method

Authors : Himanshu Singh, Rishi Kant, Shantanu Bhattacharya

Abstract : This paper adopts a top-down approach for mathematical modeling to predict the size reduction from micro to nano-scale through persistent etching. The process is simulated using a finite difference approach. Previously, various researchers have simulated the etching process for 1-D and 2-D substrates. It consists of two processes: 1) Convection-Diffusion in the etchant domain; 2) Chemical reaction at the surface of the particle. Since the process requires analysis along moving boundary, partial differential equations involved cannot be solved using conventional methods. In 1-D, this problem is very similar to Stefan's problem of moving ice-water boundary. A fixed grid method using finite volume method is very popular for modelling of etching on a one and two dimensional substrate. Other popular approaches include moving grid method and level set method. In this method, finite difference method was used to discretize the spherical diffusion equation. Due to symmetrical distribution of etchant, the angular terms in the equation can be neglected. Concentration is assumed to be constant at the outer boundary. At the particle boundary, the concentration of the etchant is assumed to be zero since the rate of reaction is much faster than rate of diffusion. The rate of reaction is proportional to the velocity of the moving boundary of the particle. Modelling of the above reaction was carried out using Matlab. The initial particle size was taken to be 50 microns. The density, molecular weight and diffusion coefficient of the substrate were taken as 2.1 gm/cm3, 60 and 10-5 cm2/s respectively. The etch-rate was found to decline initially and it gradually became constant at 0.02μ/s (1.2μ/min). The concentration profile was plotted along with space at different time intervals. Initially, a sudden drop is observed at the particle boundary due to high-etch rate. This change becomes more gradual with time due to declination of etch rate.

Keywords : particle size reduction, micromixer, FDM modelling, wet etching
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