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Numerical optimization of collisional cross sections for plasma simulation by Broyden-Fletcher-Goldfarb-Shanno method SANG-YOUNG CHUNG, DEUK-CHUL KWON, MI-YOUNG SONG, JUNG-SIK YOON, National Fusion Research Institute — For reliable plasma simulation an accurate full-set data of collision cross sections between each species participated in the plasma is required. However, the full-set of the reaction data is hard to achieve and estimated data have been used for the missing. To achieve reliable reaction data researchers have tuned the estimated reaction data so that the simulation results with the data agree with experimental results. However, as the number of data to be tuned is increased it becomes very hard work for researchers. In this study, we developed a code to optimize the data numerically based on the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm and adopted with a 0-dimensional global simulator for semiconductor processing plasma. BFGS algorithm is a type of a quasi-Newton method. The second derivatives are used for a next estimation like Newton method but are calculated by iterations from first derivatives and previous second derivatives. So the function is called (i.e. the simulator is executed) much smaller times than Newton method. Parallel algorithm was applied to the code to save time. In the serial code the calculation time for each iteration were proportional to the number of unknown variables but it became independent of the number of the variables in the parallel code.

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