Numerical Study of Nanoparticle Synthesis in Tandem-PMITP+TCFF Method with Variation of Modulation Period

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We have constructed a numerical simulation model for silicon nanoparticle synthesis using "Tandem-type Pulse Modulated Induction Thermal Plasma (Tandem-PMITP)" and "Time-Controlled Feeding of Feedstock (TCFF) method" [1][2]. The model can calculate the electromagnetic thermal-fluid fields in Tandem-PMITP, as well as the behavior of feedstock materials and the nucleation and growth of nanoparticles. In this study, we investigated the effect of modulation period on the number and size of synthesized nanoparticles using this model.

In this numerical simulation model, the thermal plasma was treated as electromagnetic thermofluid. The governing equations includes the conservation equations for mass, momentum, and energy, as well as the Poisson equation for the two vector potentials generated by the two coil currents. The SIMPLE method was adopted to solve the temperature and gas flow velocity fields. The feedstock particles were considered as Lagrangian particles, and their conservation equations for mass, momentum, and energy were solved using the 4th order Runge-Kutta method. For nanoparticle formation and transport, the aerosol general dynamic equation was solved using the method of moment (MOM). Calculation conditions were as follows. Ar gas was injected from the top of the torch as a sheath gas with a 90 L/min flow rate. Si feedstock was intermittently supplied at a rate of 1.0 g/min/rad, synchronized with the modulation cycle of the coil current, with Ar carrier gas with a 4 L/min flow rate from the water-cooled tube at the center of the torch. Fig.1 shows the relationship between the modulated coil current and the feedstock feeding phase for two conditions as examples. The lower coil current amplitude was modulated into a rectangular waveform with a 50% duty factor (DF). The modulation cycles of the lower coil current were set as T_{period} = 20 ms, 40 ms, 60 ms, 80 ms and 100 ms.

Fig. 2 shows the calculated particle size distribution in the computational domain of the reaction chamber for T_{period} = 20 ms and 80 ms. In addition, Fig. 3 indicates the relationship between the number of synthesized nanoparticles and the averaged particle diameter $\bar{d}$ for each conditions. The particle size distribution was obtained by calculating the time-averaged values of the three moments for each computational mesh and then adding the local particle size distribution for each mesh based on the geometric mean diameter and geometric mean volume. The nanoparticles with diameters less than 5 nm were ignored. As seen in these figures, an increase in modulation period from 20 ms to 80 ms elevates the nanoparticle synthesis rate by approximately 8 times. This is because the increase in low-temperature duration of the plasma due to elongating the modulation period can keep the temperature field around 2000 K, where Si nucleation becomes dominant. On the other hand, the increase in the modulation period also increases the average particle size, because the increase in the high-temperature duration of the plasma has led to easier coagulation of the generated nanoparticle nuclei.

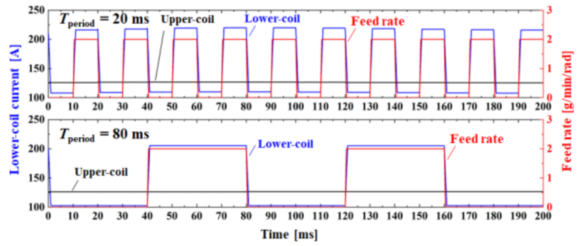

Fig. 1 : Coil current and feed rate at T_{period} = 20 ms, 80 ms.

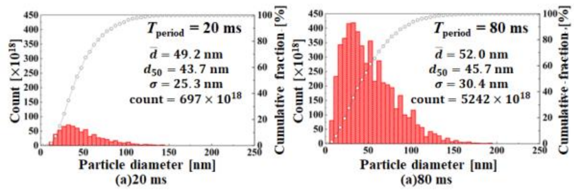

Fig. 2 : Calculated particle size distribution at T_{period} = 20 ms, 80 ms.

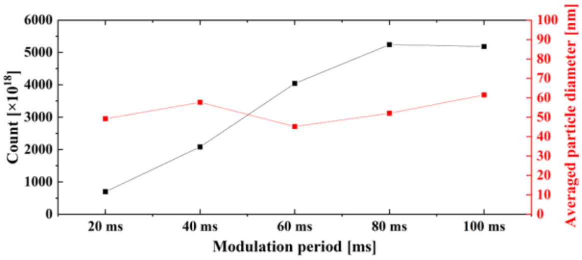

Fig. 3: Calculated nanoparticle count and mean diameter for each conditions.

References
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