Numerical Investigation for Growth Mechanisms of Ti-Based Intermetallic Nanoparticles in RF Thermal Plasmas

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MULTISCALE SIMULATION OF FUNCTIONALIZATION OF SURFACES USING ATMOSPHERIC PRESSURE DISCHARGES*

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Pulsed atmospheric pressure plasma discharges, such as corona and dielectric barrier devices, are commonly used to functionalize surfaces (e.g., polymer sheets). The surfaces of these materials have surface roughness of 100s nm to 10s μm often resulting from the manufacturing process. For example, polypropylene surfaces consist of random assemblies of crystalline strands with diameters of 100s nm. Porous materials and textiles also have highly non-planar surfaces. The penetration of plasma generated species (electrons, ions and radicals) into surface structures is of great interest when uniform functionalization of the surface is desired.

In this paper, we discuss results from a computational multiscale investigation of atmospheric pressure plasma treatment of surfaces having microstructure. The investigation was conducted with a 2-dimensional plasma hydrodynamics model using an unstructured mesh capable of resolving a dynamic range of 1000 in spatial scale.[1] This capability enables a multi-scale approach in which the reactor scale plasma hydrodynamics and penetration of plasma produced species into surface structures can be simultaneously addressed. A surface kinetics model is integrated with the plasma hydrodynamics model to assess the uniformity of treatment on the surface structures.

Investigations were preformed for discharges in atmospheric pressure air and He/O_2 mixtures, the latter being for treating surfaces when nitrogen fixing is not desired. A typical treatment geometry consists of a dielectric barrier-corona with a gap of a few mm to the surface to be treated. Surface structures have characteristic dimensions of a few μm. We found that the uniformity of treatment of polymers such as polypropylene is sensitive to the gas mixture and polarity of the discharge pulses on both macroscopic (a few mm) and microscopic (< 1 μm) scales. For example, the fraction of O_2, which in turn determines the rate of formation of O_3, can be used to optimize uniformity by controlling the rate of transport and reaction limited processes.

[1] A. N. Bhoj and M. J. Kushner, J. Phys. D. **37**, 2910 (2004)

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NUMERICAL INVESTIGATION FOR GROWTH MECHANISMS OF Ti-BASED INTERMETALLIC NANOPARTICLES IN RF THERMAL PLASMAS

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Nanoparticle synthesis with RF thermal plasmas has been proposed as an attractive material process since RF thermal plasmas have several advantages such as high enthalpy, high chemical reactivity, variable properties, large plasma volume and long residence/reaction time due to the comparatively low velocity. Furthermore, they are inherently clean since they can be generated without internal electrodes.

RF thermal plasmas are intensively useful to synthesize intermetallic nanoparticles of borides and silicides providing high electrical conductivity, heat/wear resistance and hardness. However, the synthesis includes difficult processes with vapor pressure differences. Only a few studies about the synthesis of boride and silicide nanoparticles in RF thermal plasmas have been conducted up to the present[1,2]. The growth mechanisms of Ti-based intermetallic nanoparticles of borides and silicides in RF thermal plasmas are still poorly understood. Therefore, numerical investigation was conducted for the synthesis of Ti-based intermetallic nanoparticles in an RF thermal plasma to clarify the growth mechanism for Ti-B system and Ti-Si system.

In Ti-B system, nuclei of boron are produced and grow in the upstream position, and titanium vapor subsequently condenses on the boron nanoparticles. On the other hand in Ti-Si system, silicon nucleates, and the vapors of titanium and silicon condense on the silicon nuclei simultaneously.

Critical diameters as well as homogeneous nucleation rates are strongly dependent on the supersaturation ratios and the surface tensions. The fewer nuclei with the larger sizes are produced in Ti-Si system. An amount of the vapors consumed per one nucleus to grow is larger since a smaller number of the larger nuclei are produced in Ti-Si system. As the result, the obtained particle diameters in Ti-Si system show larger than those in Ti-B system.

The boron content in the boride nanoparticles shows a wide range since condensations of titanium and boron occur at the different positions. The silicon content in the silicide nanoparticles shows a narrow range since condensations of titanium and silicon occur simultaneously.

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