3D modelling of a DC transferred arc twin torch plasma system for the synthesis of copper nanoparticles

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Abstract: An atmospheric pressure DC transferred arc twin torch thermal plasma system has been characterized by 3D simulation in order to assess its potential for the synthesis of copper nanoparticles from solid precursors. The numerical model takes into account the non-negligible effect on process temperature of radiative losses from the copper vapour. Mean diameter and yield of the synthetized nanoparticles have been investigated for different current levels, gas flow rates and precursor feed rates.

Keywords: Thermal plasmas, 3D modelling, twin torch, nanoparticle synthesis.

1. Introduction

DC transferred arc twin torch plasma systems are devices consisting of two electrodes generating a plasma arc sustained by means of an electric current flowing through the body of the discharge; this plasma arc is typically characterized by a very high temperature (20-30 kK) [1]. Twin torches are intrinsically asymmetrical systems, with cathodic and anodic electrodes having their axes tilted with respect to the vertical; the discharge generated by this particular plasma source configuration is characterized by a complex shape and fluid dynamic behaviour and a 3D description is needed in order to realistically predict it. 3D models have been previously used to study temperature and velocity distribution of such devices [2]. In this work we present a static 3D LTE model for the synthesis of copper nanoparticles in argon plasma by evaporation of micrometric solid copper precursors in a twin torch plasma system. The synthesis process occurs inside a reaction chamber, with precursors fed vertically along the axis of the chamber with a carrier gas. The precursors are vaporized by interaction with the plasma arc and nanoparticles are synthetized in the reaction chamber by interaction with a quenching gas flow rate. In a twin torch system, the strong local cooling of the plasma near the region where the material is injected in the plasma and evaporated due to radiative power losses can affect the behaviour of the arc. In order to control particle size distribution and increment the nanoparticle yield, several typologies of quenching strategies can be adopted, with different effects [3].

2. Modelling approach and results

The nanoparticle synthesis process, including plasma thermo-fluid dynamics, electromagnetic field, precursor injection and evaporation, and nanoparticle formation, transport and growth, is modelled within a 3D framework in the ANSYS FLUENT© environment.

A computational mesh of 3.8 million of polyhedral elements has been used and it is represented in Fig. 1. Electrodes' interfaces are taken into account using a simplified approach, imposing a current density distribution on the cathode surface and a zero-voltage potential on the anode. [2] The operating pressure is set to 100 kPa. Plasma thermodynamic and transport properties for pure Ar in LTE have been computed as in [4]. The physical properties for copper powders used in the implementation of the nanoparticles synthesis model [5] are reported in [3]. The feed rate of the micro-sized copper precursor particles (mean diameter = 7.3 μm) injected through the probe were assumed to have a Rosin-Rammler distribution with mean diameter of 7.3 μm.

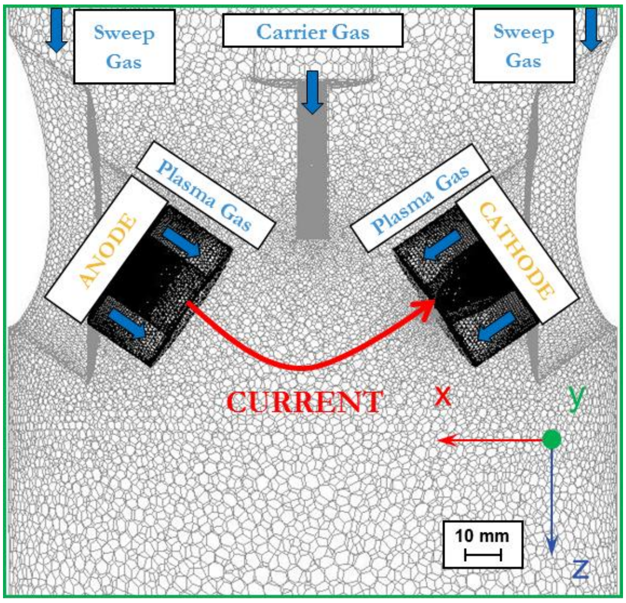

Fig. 1 Detail of the mesh in the inter-electrode and plasma discharge region.

At 520 A of operating current (Fig. 2) the evaporation efficiency is close to 70% up to 24 kg/day of precursor feed rate. Experiments performed in the Horizon 2020 INSPIRED project at 520 A show an average 67%

evaporation efficiency for ~ 0.38 kg/hr, which is in very good agreement with the output from simulation (66,5%).

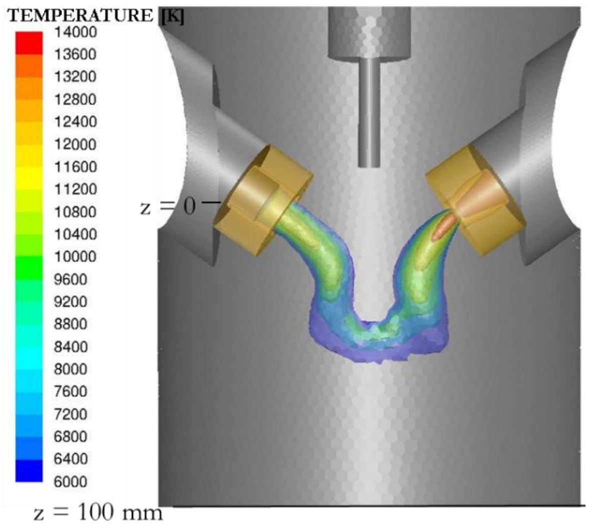

Fig. 2 Temperature isosurfaces for the case at 520 A and a precursor feed rate of 0.25 kg/h

Results of the copper nanoparticles distribution obtained using the method of moments and nodal method are shown in Fig. 33 and in Fig. 4. Nanoparticles are lost in the chamber by wall deposition. With a complete downwards flow, growth mechanisms like condensation and coagulation should increase mean particle size along the reaction chamber with a unidirectional downwards flow Vortices instead bring back upwards nanoparticles, increasing their size. **Errore. L'origine riferimento non è stata trovata.**

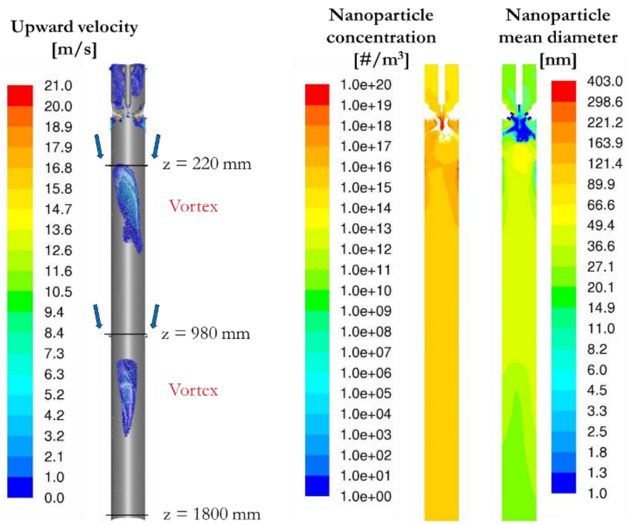

Fig. 3 Nanoparticles concentration and mean diameter in the reaction chamber with the method of moments, on the right, for the case at 520 A and a precursor feed rate of 1 kg/h. On the left, vectors of upwards velocity, showing the presence of vortices in the chamber.

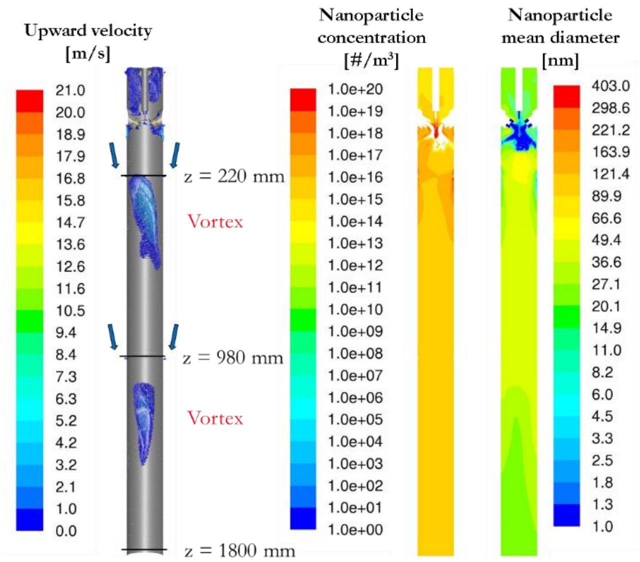

Fig. 4 Nanoparticles concentration and mean diameter in the reaction chamber with the nodal methods, on the right, for the case at 520 A and a precursor feed rate of 1 kg/h. On the left, vectors of upwards velocity, showing the presence of vortices in the chamber.

3. Conclusions

The effect of different precursor flow rate, operative current and quench gas flow rates on the nanoparticles mean diameter and yield have been investigated. The adopted simulative model can describe plasma thermo-fluid dynamics, electromagnetic fields, precursor trajectories and thermal history and nanoparticle nucleation and growth. Radiative losses from copper vapour and their effect on the precursor evaporation efficiency have also been taken into account in the model.

4. Acknowledgments

Work supported by European Union’s Horizon 2020 research and innovation program under grant agreement No 646155 (INSPIRED project).

5. References

[1] J. Heberlein and A. B. Murphy, J. Phys. D: Appl. Phys., **41**, 053001 (2008).
[2] V. Colombo, E. Ghedini, M. Boselli, P. Sanibondi and A. Concetti, J. Phys. D: Appl. Phys., **44**, 194005 (2011).
[3] S. Bianconi, M. Boselli, M. Gherardi and V. Colombo, Plasma Chem. Plasma Process., **37**, 717 (2017).
[4] V. Colombo, E. Ghedini, J. Mostaghimi, Ieee Trans. Plasma Sci. **36**, 1040 (2008).
[5] V. Colombo, E. Ghedini, M. Gherardi, P. Sanibondi, M. Shigeta, Plasma Sources Sci. Technol., **21** 025001 (2012).