COMSOL CONFERENCE ROTTERDAM 2013

Oxidation of Titanium Particles during Cold Gas Dynamic Spraying

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Cold Spray method

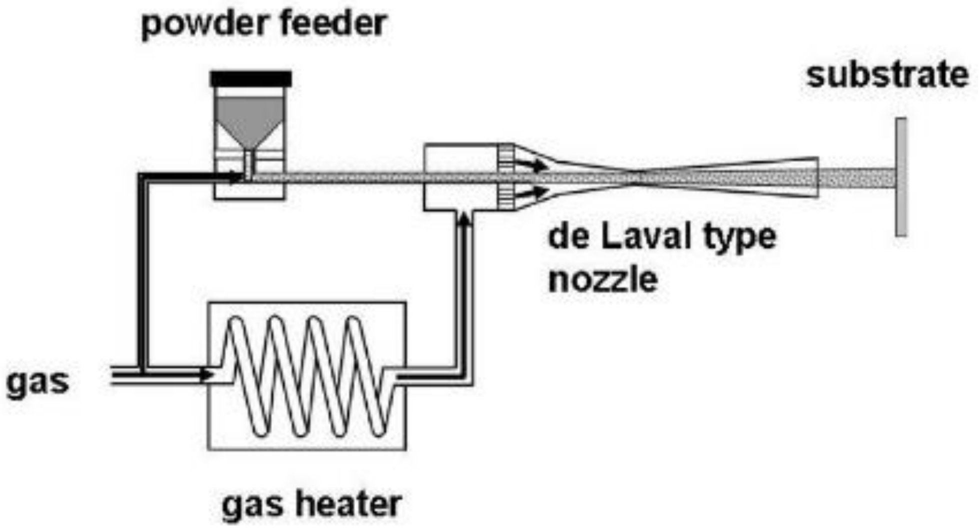
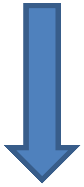


Fig 1. Schematic diagram of the cold spray process[1]

Process gases:

- Nitrogen
- Helium



AIR ?

[1]J. Voyer, T. Stoltenhoff, H. Kreye, in: C. Moreau, B. Marple (Eds.), Thermal Spray 2003: Advancing the Science & Applying the Technology, ASM International, Materials Park, OH, USA, 2003, p. 71

Oxidation model

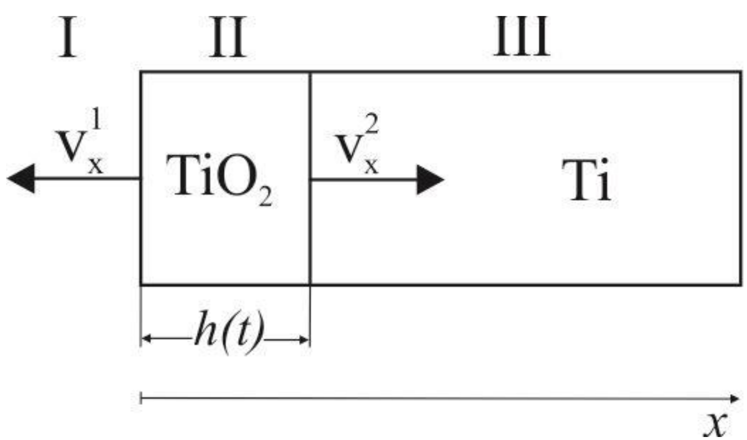
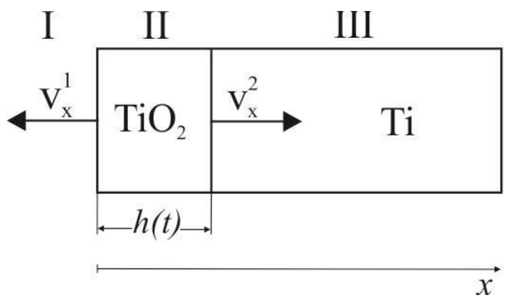


Fig 2. Schemat of 1D oxidation problem

Regions:
I - the air surrounding the sample,
II – formed titanium dioxide,
III - titanium

Entchev P. B., Lagoudas D.C. , Slattery J. C., Effects of non-planar geometries and volumetric expansion in the modeling of oxidation in titanium, International Journal of Engineering Science vol. 39, 2001, pp. 695–714

Oxidation model



- **mass balance for O_2**:

$$\frac{\partial c_{O_2}}{\partial t} - D_{(O_2,TiO_2)} \frac{\partial^2 c_{O_2}}{\partial x^2} = 0,$$

where: $D_{(O_2,TiO_2)}$ - diffusion coefficient of oxygen in titanium dioxide with following boundary conditions: $c_{O_2} = c_0 \; at \; x = 0, \;\; c_{O_2} = 0 \; at \; x = h(t)$

- **velocity of air-titanium interface (I/II):**

$$v_x^1 = -(1-\gamma) \frac{R_i}{R_0} \frac{D_{(O_2,TiO_2)}}{c_{TiO_2}} \frac{\partial c_{O_2}}{\partial x}\bigg|_{x=h(t)}$$

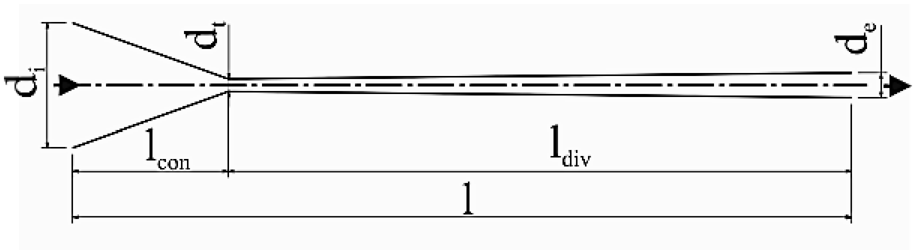
where: R_i – the length of titanium region (III), R_0 – the length of oxidized titanium region (II), γ – the Pilling-Bedworth Ratio given by equation: $\gamma \equiv \frac{c_{Ti}}{c_{TiO_2}} = \frac{\rho_{Ti}}{\rho_{TiO_2}} \frac{M_{(Ti)}}{M_{(TiO_2)}}$, c_{TiO_2}= 53.2 kmole/m^3, c_{Ti}= 93.9 kmole/m^3, c_0= 12.5 kmole/m^3

- **velocity of the oxide-titanium interface (II/III)**

$$v_x^2 = -\frac{D_{(O_2,TiO_2)}}{c_{TiO_2}} \frac{\partial c_{O_2}}{\partial x}\bigg|_{x=h(t)}$$

Entchev P. B., Lagoudas D.C. , Slattery J. C., Effects of non-planar geometries and volumetric expansion in the modeling of oxidation in titanium, International Journal of Engineering Science vol. 39, 2001, pp. 695–714

Spraying parameters



Powder injection	d_i [mm]	d_t [mm]	d_e [mm]	l [mm]	l_{con} [mm]	l_{div} [mm]
axial	40	2	4	250	50	200

- **Velocity of powder particles:**

$$m_p \cdot \frac{dv_p}{dt} = \frac{3}{4}\frac{C_D}{D_p}\frac{\rho_g}{\rho_p}(v_g - v_p)|v_g - v_p|$$

Where: C_D is the drag coefficient , v_p is particle velocity, v_g is gas velocity, ρ_p – density of particle material, ρ_g – density of gas

- **Temperatures of powder particles**

$$\frac{dT_p}{dt} = v_p \cdot \frac{dT_p}{dx} = (T_g - T_p)\frac{6h}{c_{pp}\rho_p D_p}$$

where, T_p is particle temperature, T_g is gas temperature, c_{pp} is heat capacity of particle, v_p is particle velocity, C_{pg} is heat capacity, h is heat transfer coefficient related to the thermal conductivity of gas by Nusselt number (Nu)

Victor K. Champagne The Cold Spray Materials Deposition Process: Fundamentals and Applications, Woodhead Publishing Limited, 2007

Spraying parameters

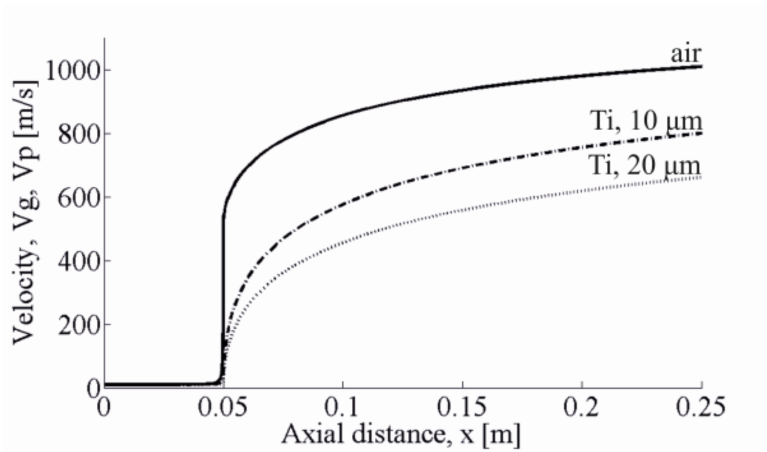


Fig 3. Titanium particles velocity during cold spraying

Particle's residence time in the nozzle ~0.0052 s.

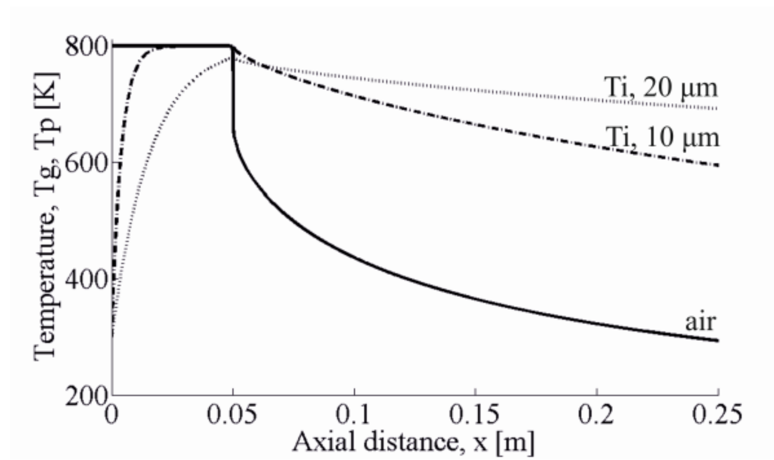


Fig 4. Titanium particles temperature during cold spraying

Diffusion coefficient[2]:

$$D_{(O_2,TiO_2)} = 870\ \exp(-\frac{55535}{RT})$$

[2]Christoulis D.K., Guetta S., Guipont V., Jeandin M., The Influence of the Substrate on the Deposition of Cold-Sprayed Titanium: An Experimental and Numerical Study, Journal of Thermal Spray Technology, vol. 20(3) , 2011, pp. 523–533

Results

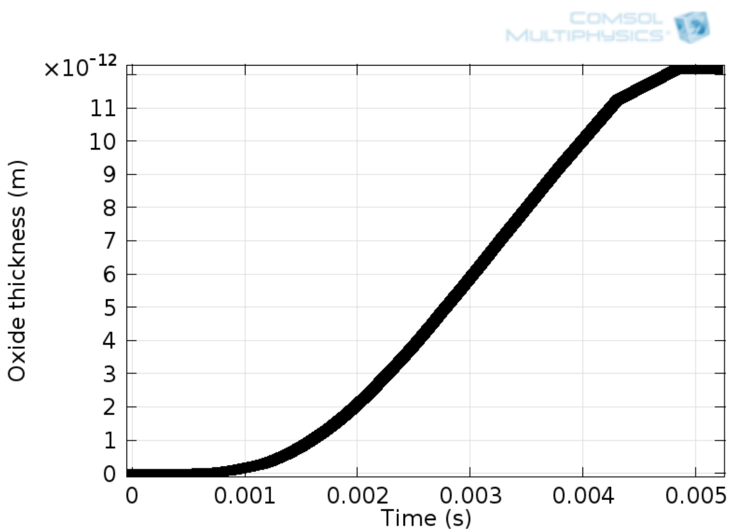


Fig 5. Oxide thickness grow during residence time in nozzle for particle 10 µm

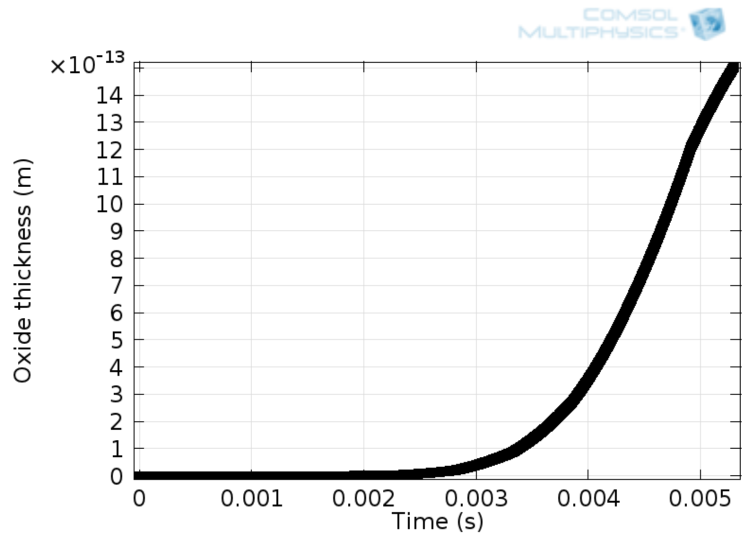


Fig 6. Oxide thickness grow during residence time in nozzle for particle 20 µm

Conclusions

- oxide formation during the residence time in nozzle is negligible
- oxygen dissolution in titanium as well as the possibility of damage to the oxide layer may have an effect on the final oxidation of the sprayed coating
- long contact time between the air stream issuing from the nozzle and forming coating may cause an increase in oxide content

Thank you for your attention