Numerical modelling of chemo-mechanical degradation of historical oil paintings

Gerardus J.A.M. Eumelen*, **Emanuela Bosco and Akke S.J. Suiker**

Department of the Built Environment,
Eindhoven University of Technology,
P.O. Box 513, 5600 MB Eindhoven, The Netherlands
email: g.j.a.m.eumelen@tue.nl

ABSTRACT

In this work, a computational chemo-mechanical model is proposed that aims at describing the complex degradation process of historical oil paintings due to metal soap formation and growth. Oil paintings consist of layers that contain an oil binding medium with metal-based pigment particles embedded. Metal soaps form from chemical diffusion and reaction of saturated fatty acids - which are a degradation product of the oil binder - with metal ions released by the pigments [1]. Metal soap formation may result into large crystals with an average size of $100 - 200$ μm, which can protrude through the paint surface, with negative consequences for its visual appearance. Additionally, metal soaps may promote cracking and flaking of paint layers [2].

The chemical process of metal soap formation and growth is simulated by a diffusion-reaction model, in which the saturated fatty acids are considered as the reference diffusing species. The growth of a metal soap crystal is simulated by introducing a small reaction zone on the boundary of a predefined metal soap nucleus. Once a material point within the reaction zone is crystallized, the boundary of the crystal changes, thereby advancing the reaction zone. The formation of the metal soap crystal introduces expansive strains (and therefore stresses) in the domain, which can ultimately lead to crack nucleation and propagation. These processes are modelled by means of a discrete crack formulation based on cohesive zones [3], using interface elements equipped with a traction-separation law [4]. The cohesive zone model has also been implemented in the diffusion-reaction model, in order to reduce the mass-flux of saturated fatty acids when the damage across the crack faces increases.

The coupled chemo-mechanical model has been implemented within the finite element framework using a staggered approach. Results from the numerical analyses show that the model is capable of simulating the growth of a metal soap crystal and the consequent onset of damage. The simulated surface deflection of the paint layer shows to be in good qualitative agreement with cross-sectional observations from real paintings. Furthermore, a parameter variation study performed on different chemical and mechanical parameters illustrates their influence on the growth of the metal soap crystal and the damage formation in the paint layer.

REFERENCES

[1] Hermans, J.J., Keune, K., Van Loon, A., Iedema, P.D. The crystallization of metal soaps and fatty acids in oil paint model systems. *Physical Chemistry Chemical Physics.* (2016) **18**:10896–10905.

[2] Boon, J.J., Van der Weerd, J., Keune, K., Noble, P., Wadum, J. Mechanical and chemical changes in Old Master paintings: dissolution, metal soap formation and remineralization processes in lead pigmented ground/intermediate paint layers of 17th century painting. *13th Triannial meeting of the ICOM committee for conservation in Rio De Janero.* (2002) **Vol. I**:401–406.

[3] Xu, X.-P., Needleman, A. Numerical simulations of fast crack growth in brittle solids. *Journal of the Mechanics and Physics of Solids.* (1992) **42**:1397–1434.

[4] Cid Alfaro, M.V., Suiker, A.S.J., De Borst, R., Remmers, J.J.C. Analysis of fracture and delamination in laminates using 3D numerical modelling. *Engineering Fracture Mechanics* (2009) **76**:761–780