



HAL
open science

Modélisation multiphysique d'une interface adhésive : dommage mécanique et réactions chimiques

Sébastien d'Andréa, Stéphane Lejeunes, Frédéric Lebon, Victor Blanc, Marc
Lainet, Thomas Helfer

► To cite this version:

Sébastien d'Andréa, Stéphane Lejeunes, Frédéric Lebon, Victor Blanc, Marc Lainet, et al.. Modélisation multiphysique d'une interface adhésive : dommage mécanique et réactions chimiques. 25e Congrès Français de Mécanique, Nantes, 29 août-2 septembre 2022, Aug 2022, Nantes, France. hal-04281719

HAL Id: hal-04281719

<https://hal.science/hal-04281719>

Submitted on 13 Nov 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Multiphysics modeling of adhesive interface with damage

S. D'andréa¹, S. Lejeunes², F. Lebon², V. Blanc¹, M. Lainet¹, T. Helfer¹

1.CEA/DES/IRESNE/DEC, Cadarache F 13108 St Paul Lez Durance,
{Sebastien.DANDREA,victor.blanc,marc.lainet,thomas.helfer}@cea.fr

2. Aix-Marseille Univ, CNRS, Centrale Marseille, LMA, {lejeunes,lebon}@lma.cnrs-mrs.fr

Abstract :

In the context of fuel-cladding interaction modelling in fast nuclear reactors, a multiphysics cohesive zone model of an adhesive interface with damage is proposed. In this work, only traction/compression behaviour is described with this model. In traction, the model takes into account an elastic-brittle behaviour with temperature and adhesive links formation dependency. In compression, the model includes solid-solid contact. The effects of temperature, mechanical state, damage and chemical reactions are incorporated in adhesive links modelling. Thermal conductivity is affected by damage.

Keywords : Adhesive interface, Multiphysics, Damage

1 Introduction

In the considered fast reactor fuel element, cylindrical fuel pellets (mixed oxide $UPuO_2$) are nested inside their cladding, made of stainless steel. Pellets are initially separated from their cladding by a small radial gap of about $100 \mu\text{m}$ that can be closed during irradiation because of physical, mechanical and chemical phenomena activated by the very high temperature level (up to $2000 \text{ }^\circ\text{C}$) imposed on pellets and cladding.

On one hand, an adhesive phenomenon can be observed at this interface after irradiation under specific conditions: a minimum contact time between pellet and cladding, a temperature gradient between 500 and $700 \text{ }^\circ\text{C}$, a closed gap with a low contact pressure (about 10 MPa), the presence of fission products and a corrosion layer [1]. On the other hand, different power cycles imposed stresses at the interface can lead to a rupture of the adhesive interface (loss of contact), new adhesive interface formation (after a previous rupture) and damage (which modifies the interface physico-chemical state). Regarding the nuclear reactor safety, adhesive phenomenon modelling and his implementation in fast fuel performance code (GERMINAL) are required.

We propose here a multiphysics approach to model this adhesive interface. We are particularly interested in mechanical damage and thermochemical effects. We assume that pellet and cladding are bonded by chemical adhesion (ionic-covalent bonds). And this bonding is created by phase change of stainless steel grains in contact with oxide fuel. Phase change of stainless steel grains is motivated by chemical diffusion and reaction with oxygen and corrosive species, temperature and strain imposed by pellet cladding interaction.

Thermo-chemo-mechanical solid models are particularly studied in concrete [2, 3, 4], biological, electrical batteries [5] and inelastic solids [6] domains. In most of cases, the coupling needs between physics is justified by

the diffusion phenomenon. Diffusion can change the microstructural state: swelling, phases change and creation or repair lacuna (crystal defect) that directly modify the mechanical and thermal behaviour. All these studies take into account the diffusion phenomenon.

In [5, 7] diffusion effects on heat generation and mechanical state (change stresses) are proposed. In [2, 5, 6] the stress/strain solution of the swelling created by diffusion is studied. In [2] damage created by phase change due to diffusion is considered.

In terms of adhesive and damage interface, some studies treat the cohesive or adhesive failure with initial condition that adhesive energy is already at the maximum. They are not interested in modelling adhesive energy increase. Only studies on continuum damage-healing mechanics [8, 9] consider both adhesive energy increase and damage at a solid interface. In these works, healing is always allowed by polymers' presence at the interface and movement capacity of polymer chains [10, 11]. [12] can be cited as a case where adhesive energy is activated by distance (Van der Waals theory).

In this approach, the model take into account an adhesive interface with continuum mechanical damage, a theoretical adhesive energy higher than examples of the previously cited studies and an adhesive phenomenon activated by thermo-chemo-mechanical conditions. The mechanical behaviour depends on chemical reactions and temperature. On top of that, we propose to take oxidation and phase change models of steels to explain chemical bonds evolution.

2 Constitutive modeling

In consistency with [13, 14], we assume that the cohesive zone behaves like a standard generalized material. We first consider the case of a 1D interface i.e. an interface with only a traction/compression behaviour. We adopt a continuum point of view in the modeling of the finite-thickness interface. The normal displacement jump and the associated normal traction are denoted by U_n and t_n , respectively. To distinguish between traction and compression we assume that the normal displacement jump can be decomposed in a additive manner into extension, U_n^+ and compression, U_n^- .

To describe the oxidation phenomena and the creation of chemical adhesive bonds through the interface we introduce an internal variable, $\xi \in [0, 1]$, that corresponds to the relative percentage of chemical links ($\xi = 0$ means the absence of chemical bonds and $\xi = 1$ corresponds to 100% among all possible chemical bonds). The damage of the interface, i.e. the destruction of chemical bonds due to mechanical strain or stress, is described with the internal variable d that also varies in $[0, 1]$ ($d = 0$ means no damage).

The Helmholtz free energy, ψ , is assumed to be additively divided into a a chemical part ψ_c , a mechanical part in traction ψ_m^+ and a mechanical part in compression ψ_m^- part such as :

$$\psi(U_n, \Theta, \xi, d) = \psi_c(\xi, \Theta) + \psi_m^+(U_n^+, \Theta, \xi, d) + \psi_m^-(U_n^-, \Theta) \quad (1)$$

where Θ is the interface temperature.

For the mechanical part we adopt a linear elastic behavior for the compression and traction but we assume that only the traction behavior is sensitive to damage and chemical evolution (initially the stiffness in traction is null, there is no damage and the compression stiffness is equal to the stiffness of the neighborhood of the interface):

$$\rho\psi_m^+(U_n^+, \Theta, \xi, d) = (1-d)^2 K^+(\xi, \Theta) \frac{(U_n^+)^2}{2} \quad (2)$$

$$\rho\psi_m^-(U_n^-, \Theta) = K^- \frac{(U_n^-)^2}{2} \quad (3)$$

where K^+ and K^- are the stiffness for traction and compression respectively. K^+ depends on temperature and chemical links such as :

$$K^+(\xi, \Theta) = K\xi \exp -\frac{\Theta - \Theta_0}{\Theta_0} \quad (4)$$

where Θ_0 is the reference temperature. The last contribution is the chemical free energy. As we do not have a detailed knowledge of the reactive scheme we adopt a phenomenological point of view. The chemical reactions are simply modeled with the following energy:

$$\rho\psi_c = C \frac{(1-\xi)^{n+1}}{n+1} - \frac{C}{n+1} \quad (5)$$

where n and C are chemical parameters.

With these thermodynamic potentials, we assume that the interface does not store thermal energy. The thermal energy is just used to describe chemical reactions.

Knowing the expression of the free energy, we can write the total dissipation ϕ using the Clausius-Duhem inequality:

$$\phi = t_n \dot{U}_n - \rho \dot{\psi} - \rho s \dot{\Theta} - \frac{1}{\Theta} q_n \frac{\partial \Theta}{\partial x} \geq 0 \quad \forall q_n, \dot{U}_n, \dot{\Theta} \quad (6)$$

where ρ is the density of the interface, t_n is the normal stress, Θ is the absolute temperature, s is the local entropy and q_n is the normal thermal flux. The time derivative of the free energy is given by the following terms:

$$\rho \dot{\psi}_m^+ = (1-d)^2 K^+ U_n^+ \dot{U}_n^+ - (1-d) U_n^{+2} K^+ \dot{d} + (1-d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} \dot{\xi} + (1-d)^2 \frac{\partial K^+}{\partial \Theta} \frac{(U_n^+)^2}{2} \dot{\Theta} \quad (7)$$

$$\rho \dot{\psi}_m^- = K^- U_n^- \dot{U}_n^- \quad (8)$$

$$\rho \dot{\psi}_c = -C(1-\xi)^n \dot{\xi} \quad (9)$$

Introducing eqs. (7)-(9) in eq. (6), one can obtain:

$$\begin{aligned} \phi = & (t_n^+ - (1-d)^2 K^+ U_n^+) \dot{U}_n^+ + (t_n^- - K^- U_n^-) \dot{U}_n^- - \\ & \left((1-d)^2 \frac{\partial K^+}{\partial \Theta} \frac{(U_n^+)^2}{2} + \rho s \right) \dot{\Theta} \\ & + \left((1-d) U_n^{+2} K^+ \right) \dot{d} - \left((1-d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} - C(1-\xi)^n \right) \dot{\xi} - \\ & \frac{1}{\Theta} q_n \frac{\partial \Theta}{\partial x} \end{aligned} \quad (10)$$

The mechanical behavior is assumed to be elastic therefore we obtain the following constitutive equations for the stress:

$$t_n^+ = (1-d)^2 K^+ U_n^+ \quad (11)$$

$$t_n^- = K^- U_n^- \quad (12)$$

$$t_n = t_n^+ + t_n^- \quad (13)$$

From eq. (10) we also obtain a constitutive equation for the entropy:

$$s = -(1-d)^2 \frac{\partial K^+}{\partial \Theta} \frac{(U_n^+)^2}{2\rho} \quad (14)$$

For the normal thermal flux, we consider a standard Fourier law but affected by the damage: a fully damaged interface can not transfer heat by conduction mechanisms

$$q_n = -k_t(1-d) \frac{\partial \Theta}{\partial x} \quad (15)$$

It remains two terms in the total dissipation, one associated to damage and the other one associated to the creation of chemical bonds, eq. (10) becomes:

$$\overbrace{\left((1-d)U_n^{+2}K^+ \right)}^{A_d} \dot{d} + \overbrace{\left(-(1-d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} + C(1-\xi)^n \right)}^{A_\xi} \dot{\xi} \geq 0 \quad \forall \dot{d}, \dot{\xi} \quad (16)$$

The evolution of the damage is assumed to be of the following form:

$$\dot{d} = \frac{1}{\eta} \langle A_d - g_c d \rangle = \frac{1}{\eta} \left\langle (1-d)U_n^{+2}K^+ - g_c d \right\rangle \quad (17)$$

where η is a viscosity parameter and g_c is a critical fracture energy (MPa). For the chemical evolution we adopt the following form:

$$\dot{\xi} = a(\Theta)(1-d) \langle A_\xi \rangle = a(\Theta)(1-d) \left\langle -(1-d)^2 \frac{\partial K^+}{\partial \xi} \frac{(U_n^+)^2}{2} + C(1-\xi)^n \right\rangle \quad (18)$$

the term $a(\Theta) = A_m \exp(-E_a/(R\Theta))$ is an Arrhenius like term with E_a an activation energy, R the perfect gaz constant and A_m a kinetic factor. Introducing eqs. (17)-(18) into eq. (16) it can be seen that the Clausius-Duhem inequality is always satisfied. From eq. (18) indicate the chemical affinity (thermodynamical force associated to a chemical evolution) can be negative in tension which leads to a null chemical evolution rate. The coupling between mechanical state and chemical reaction is controlled with the help of the parameter C .

3 Model behaviour under thermal and mechanical cycles

To analyse model behaviour we propose to impose thermal and displacement cycles as shown in figures 1 and 2. The model has been implemented in the open-source MFront code generator [15, 16] and we simulate the behaviour of a material point with MTest (a code delivered with MFront).

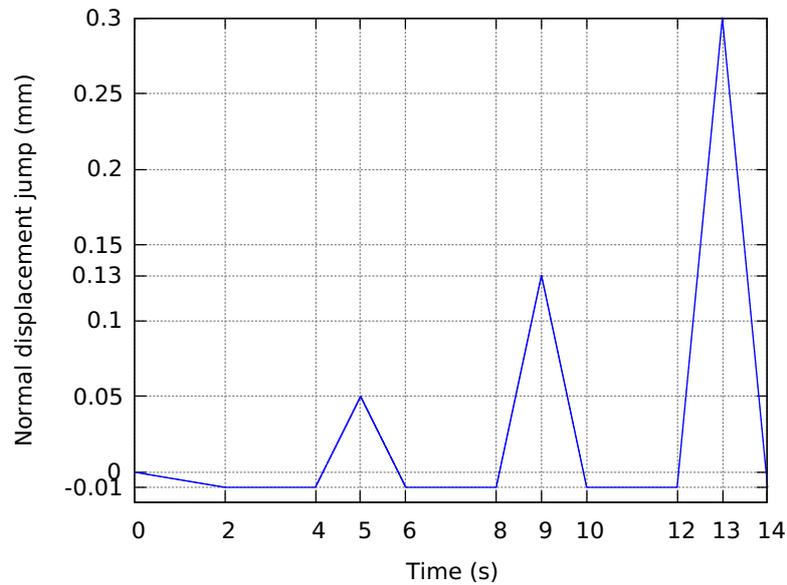


Figure 1: Normal opening displacement imposed versus time

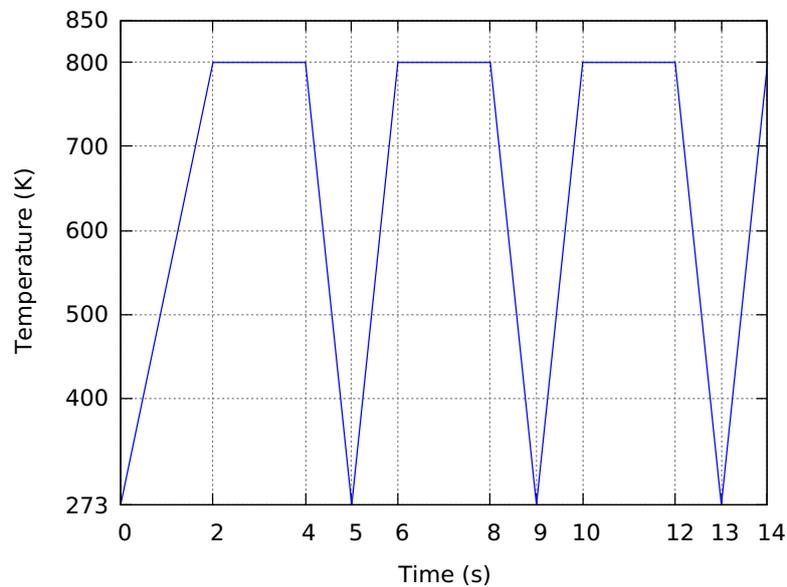


Figure 2: Temperature imposed versus time

Figure 3 shows that chemical links can't be created in traction and can increase over time in compression or null state. Temperature affects chemical links like threshold effect. Damage is similar to literature on continuum damage theory.

In figure 4 elastic-brittle behaviour is found with a stress response which depends on damage, temperature and chemical links.

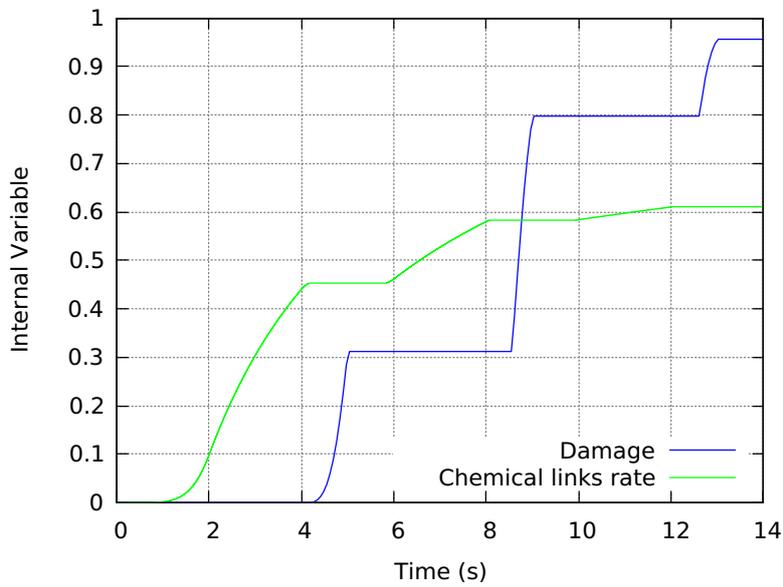


Figure 3: Internal variable evolution under cycles

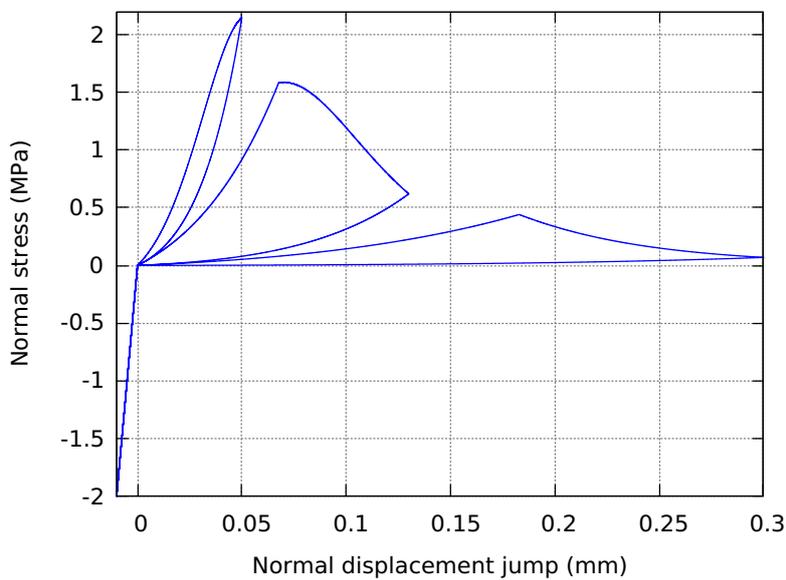


Figure 4: Model normal stress - normal displacement response under thermal and mechanical cycles

4 Adhesive contact finite elements simulation in 1, 2 or 3 dimensions

The model described in this work has been built to simulate an adhesive contact between the pellet and his cladding ,especially in 1 and 2 dimensions, with finite element method. To simulate pellet cladding adhesive interface described in the introduction 1, we consider using an adhesive contact law with this multiphysics cohesive zone. We propose to add a cohesive zone to cladding mesh frontier as well as a cohesive contact law between cohesive zone and pellet mesh. The adhesive contact law only manages contact detection and links degree of freedom of cohesive zone and pellet mesh frontier. As for the cohesive zone, it links mechanically pellet and cladding , i.e it models solid-solid contact in closed gap and adhesive behaviour in opening gap.

5 Conclusion

This work presents a thermo-chemo-mechanical model of adhesive and damage interface based on an original approach that takes into account the coupling between the three physics on traction/compression interface behaviour. Thermodynamic potential defined in this model seems to be easily adapted to model adhesive phenomenon that appears in solid-solid interface under temperature, contact pressure and corrosion. The perspective of this work is to reach a complete healing behaviour under cycles and to integrate the influence of compressive strain on chemical links evolution.

Acknowledgements

This research is conducted through collaboration between the CEA and LMA in MISTRAL laboratory and financed in the frame of the CINNA project.

References

- [1] Fitriana Nindiyasari, M. Kolluri, S. van Til, R. Hania, T. Bakker, and A. de Jong. Hot cell setup for pellet cladding interface investigation. Aix-en-Provence, October 2019.
- [2] Fadi Althoey, Paul Stutzman, Michael Steiger, and Yaghoob Farnam. Thermo-chemo-mechanical understanding of damage development in porous cementitious materials exposed to sodium chloride under thermal cycling. *Cement and Concrete Research*, 147:106497, September 2021.
- [3] Miguel Cervera, Javier Oliver, and Tomás Prato. Thermo-Chemo-Mechanical Model for Concrete. II: Damage and Creep. *Journal of Engineering Mechanics*, 125(9):1028–1039, September 1999. Publisher: American Society of Civil Engineers.
- [4] Miguel Cervera, Javier Oliver, and Tomás Prato. Thermo-Chemo-Mechanical Model for Concrete. I: Hydration and Aging. *Journal of Engineering Mechanics*, 125(9):1018–1027, September 1999. Publisher: American Society of Civil Engineers.
- [5] A. Nateghi and M.-A. Keip. A thermo-chemo-mechanically coupled model for cathode particles in lithium-ion batteries. *Acta Mechanica*, 232(8):3041–3065, August 2021.
- [6] Ignacio Romero, Eva M. Andrés, and Ángel Ortiz-Toranzo. Variational updates for general thermo-chemo-mechanical processes of inelastic solids. *Computer Methods in Applied Mechanics and Engineering*, 385:114013, November 2021.

- [7] T. I. Zohdi. Modeling and simulation of a class of coupled thermo-chemo-mechanical processes in multiphase solids. *Computer Methods in Applied Mechanics and Engineering*, 193(6):679–699, February 2004.
- [8] Ever J. Barbero, Fabrizio Greco, and Paolo Lonetti. Continuum Damage-healing Mechanics with Application to Self-healing Composites. *International Journal of Damage Mechanics*, 14(1):51–81, January 2005. Publisher: SAGE Publications Ltd STM.
- [9] Chahmi Oucif and Luthfi Muhammad Mauludin. Continuum Damage-Healing and Super Healing Mechanics in Brittle Materials: A State-of-the-Art Review. *Applied Sciences*, 8(12):2350, December 2018. Number: 12 Publisher: Multidisciplinary Digital Publishing Institute.
- [10] Ammar A. Alshegri and Rashid K. Abu Al-Rub. Finite element implementation and application of a cohesive zone damage-healing model for self-healing materials. *Engineering Fracture Mechanics*, 163:1–22, September 2016.
- [11] Chahmi Oucif, George Z. Voyiadjis, and Timon Rabczuk. Modeling of damage-healing and nonlinear self-healing concrete behavior: Application to coupled and uncoupled self-healing mechanisms. *Theoretical and Applied Fracture Mechanics*, 96:216–230, August 2018.
- [12] Mathieu Schryve. *Modèle d'adhésion cicatrisante et applications au contact verre/élastomère*. Thèse, Mécanique des Solides, Université de Provence - Aix-Marseille I, November 2008.
- [13] F. Costanzo and D. H. Allen. A continuum thermodynamic analysis of cohesive zone models. *International Journal of Engineering Science*, 33(15):2197–2219, December 1995.
- [14] Fabien Cazes, Michel Coret, Alain Combescure, and Anthony Gravouil. A thermodynamic method for the construction of a cohesive law from a nonlocal damage model. *International Journal of Solids and Structures*, 46(6):1476–1490, March 2009.
- [15] Thomas Helfer, Bruno Michel, Jean-Michel Proix, Maxime Salvo, Jérôme Sercombe, and Michel Casella. Introducing the open-source mfront code generator: Application to mechanical behaviours and material knowledge management within the PLEIADES fuel element modelling platform. *Computers & Mathematics with Applications*, 2015.
- [16] CEA and EDF. MFront Web Site, <https://thelfer.github.io/xfel/web/index.html>, 2022.