Évolution des microstructures et comportement élastoviscoplastique des matériaux

Approche phénoménologique par la théorie des champs de phase

Syllabus

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applications récentes (Schmidt et al., 2021; Pinomaa et al., 2022; Lindroos et al., 2022)

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Références

Abrivard G., Busso E.P., Forest S., and Appolaire B. (2012a). *Phase field modelling of grain boundary motion driven by curvature and stored energy gradients. Part I : theory and numerical implementation.* Philosophical Magazine, vol. 92, pp 3618–3642.

Abrivard G., Busso E.P., Forest S., and Appolaire B. (2012b). *Phase field modelling of grain boundary motion driven by curvature and stored energy gradients. Part II : Application to recrystallisation.* Philosophical Magazine, vol. 92, pp 3643–3664.

Admal N. Chandra, Po G., and Marian J. (2018). *A unified framework for polycrystal plasticity with grain boundary evolution.* International Journal of Plasticity, vol. 106, pp 1 – 30.

Admal N. C., Segurado J., and Marian J. (2019). *A three-dimensional misorientation axis- and inclination-dependent Kobayashi-Warren-Carter grain boundary model.* Journal of the Mechanics and Physics of Solids, vol. 128, pp 32 – 53.

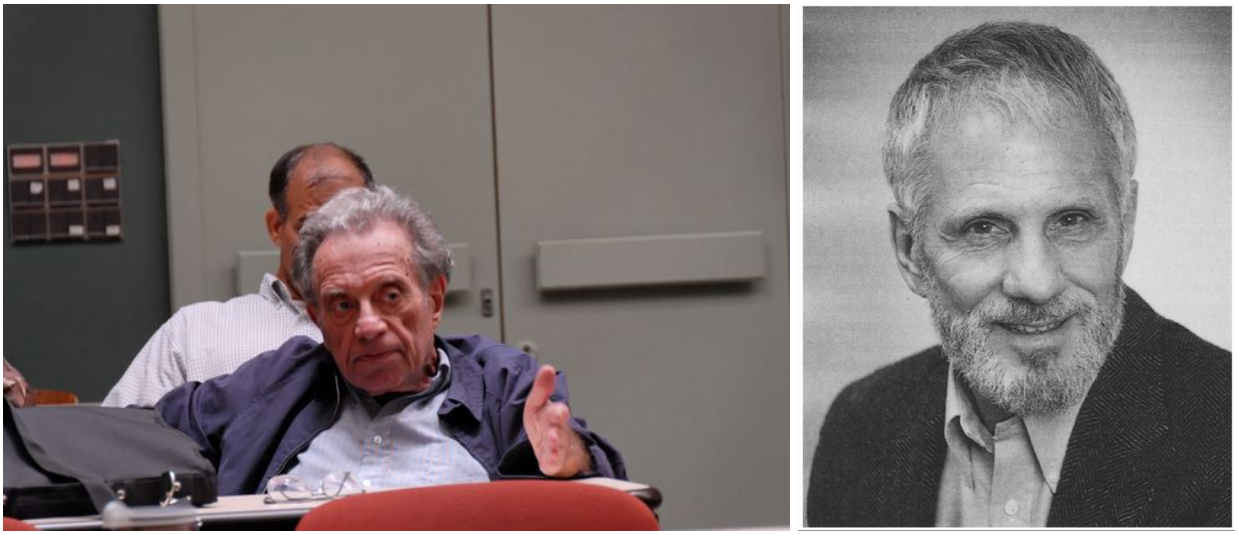

FIGURE 1 – Bernard D. Coleman (1930-) à Paris (CMDS11, 2007), Morton E. Gurtin (1934-2022).

FIGURE 2 – Gordon school 1974 : John Werner Cahn (Cologne 1928-2016 Seattle, MIT-NIST), Francis C. Larché, André Pineau...

FIGURE 3 – Die 3 Wolfgangs : Wolfgang Müller, Wolfgang Muschik, Wolfgang Dreyer, 2003 (Institut fü Mechanik, Institut für Theoretische Physik, WeierstraaInstitut, Berlin).

FIGURE 4 – La coopération avec Benoît Appolaire (ONERA puis Université de Lorraine) et Kais Ammar (Mines Paris).

Ammar K., Appolaire B., Cailletaud G., Feyel F., and Forest S. (2009a). *Finite element formulation of a phase field model based on the concept of generalized stresses.* Computational Materials Science, vol. 45, pp 800–805.

Ammar K., Appolaire B., Cailletaud G., and Forest S. (2009b). *Combining phase field approach and homogenization methods for modelling phase transformation in elastoplastic media.* European Journal of Computational Mechanics, vol. 18, pp 485–523.

Ammar K., Appolaire B., Cailletaud G., and Forest S. (2011). *Phase field modeling of elasto-plastic deformation induced by diffusion controlled growth of a misfitting spherical precipitate.* Philosophical Magazine Letters, vol. 91, pp 164–172.

Ammar K., Appolaire B., and Forest S. (2021). *Splitting of dissolving precipitates during plastic shear : A phase field study.* Comptes Rendus. Physique, vol. 22, pp 353–370.

Ammar K., Appolaire B., Forest S., Cottura M., Le Bouar Y., and Finel A. (2014). *Modelling inheritance of plastic deformation during migration of phase boundaries using a phase field method.* Meccanica, vol. 49, pp 2699–2717.

Ask A., Forest S., Appolaire B., and Ammar K. (2018a). *Cosserat crystal plasticity with dislocation–driven grain boundary migration.* Journal of Micromechanics and Molecular Physics, vol. 3, pp 1840009.

Ask A., Forest S., Appolaire B., and Ammar K. (2019). *A Cosserat–phase field theory of crystal plasticity and grain boundary migration at finite deformation.* Continuum Mechanics and Thermodynamics, vol. 31, pp 1109–1141.

Ask A., Forest S., Appolaire B., and Ammar K. (2020). *Microstructure evolution in deformed polycrystals predicted by a diffuse interface Cosserat approach.* Advanced Modeling and Simulation in Engineering Sciences, vol. 7 n° 9.

Ask A., Forest S., Appolaire B., Ammar K., and Salman O. U. (2018b). *A Cosserat crystal plasticity and phase field theory for grain boundary migration.* Journal of the Mechanics and Physics of Solids, vol. 115, pp 167–194.

Bartels Alexander and Mosler Jörn (2017). *Efficient variational constitutive updates for Allen–Cahn-type phase field theory coupled to continuum mechanics.* Computer Methods in Applied Mechanics and Engineering, vol. 317, pp 55 – 83.

Borukhovich E., Engels P.S., Boehlke T., Shchyglo O., and Steinbach I. (2014). *Large strain elasto-plasticity for diffuse interface models.* Modelling and Simulation in Materials Science and Engineering, vol. 22.

Borukhovich Efim, Engels Philipp S., Mosler Jörn, Shchyglo Oleg, and Steinbach Ingo (2015). *Large deformation framework for phase-field simulations at the mesoscale.* Computational Materials Science, vol. 108, pp 367 – 373.

Cahn J.W. and Hilliard J.E. (1958). *Free energy of a Nonuniform system. I. Interfacial free energy.* The Journal of Chemical Physics, vol. 28, pp 258–267.

Cahn J. and Larché F. (1985). *The Interactions of Composition and Stress In Crystalline Solids.* Acta Metallurgica, vol. 33, pp 331–357.

Chatterjee S., Schwen D., and Moelans N. (2022). *An efficient and quantitative phase-field model for elastically heterogeneous two-phase solids based on a partial rank-one homogenization scheme.* International Journal of Solids and Structures, vol. 250, pp 111709.

Cottura M., Appolaire B., Finel A., and Bouar Y. Le (2016). *Coupling the Phase Field Method for diffusive transformations with dislocation density-based crystal plasticity : Application to Ni-based superalloys.* Journal of the Mechanics and Physics of Solids, vol. 94, pp 473 – 489.

Cottura M., Le Bouar Y., Finel A., Appolaire B., Ammar K., and Forest S. (2012). *A phase field model incorporating strain gradient viscoplasticity : application to rafting in Ni-base superalloys.* Journal of the Mechanics and Physics of Solids, vol. 60, pp 1243–1256.

de Groot S.R. and Mazur P. (1962–1984). *Non–equilibrium thermodynamics.* North Holland–Dover.

Dreyer W. and Müller W.H. (2000). *A study of the coarsening in tin/lead solders.* International Journal of Solids and Structures, vol. 37, pp 3841–3871.

Dreyer W. and Müller W.H. (2001). *Modeling diffusional coarsening in eutectic tin/lead solders : A quantitative approach.* Int. J. Solids Structures, vol. 38, pp 1433–1458.

Durga A., Wollants P., and Moelans N. (2013). *Evaluation of interfacial excess contributions in different phase-field models for elastically inhomogeneous systems.* Modelling and Simulation in Material Science and Engineering, vol. 21, pp 055018.

Durga A., Wollants P., and Moelans N. (2015). *A quantitative phase–field model for two–phase elastically inhomogeneous systems.* Computational Materials Science, vol. 99, pp 81–95.

Fandeur O., Helfer T., Siedel D., Ammar K., and Forest S. (2022). *Une approche micromorphe de l'endommagement de matériaux quasi-fragiles : implémentation numérique et lien avec la méthode par champ de phase.* In : 15ème colloque national en calcul des structures, Hyères-les-Palmiers, France.

Finel A., Le Bouar Y., Gaubert A., and Salman U. (2010). *Phase field methods : Microstructures, mechanical properties and complexity.* Comptes Rendus Physique, vol. 11, pp 245–256.

Forest S. (2008). *The micromorphic approach to plasticity and diffusion.* In : Continuum Models and Discrete Systems CMDS11, eds. Jeulin D. and Forest S., pp 105–112. Mines Paris Les Presses.

Forest S. (2009). *The micromorphic approach for gradient elasticity, viscoplasticity and damage.* ASCE Journal of Engineering Mechanics, vol. 135, pp 117–131.

Forest S. (2018). *Use and Abuse of the Method of Virtual Power in Generalized Continuum Mechanics and Thermodynamics.* In : Generalized Models and Non-classical Approaches in Complex Materials 1, eds. Altenbach H., Pouget J., Rousseau M., Collet B., and Michelitsch T., pp 311–334. Springer International Publishing.

Forest S., Ammar K., and Appolaire B. (2011). *Micromorphic vs. phase–field approaches for gradient viscoplasticity and phase transformations.* In : Advances in Extended and Multifield Theories for Continua, ed. Markert B., pp 69–88. Lecture Notes in Applied and Computational Mechanics 59, Springer.

Forest S., Ammar K., Appolaire B., Cordero N.M., and Gaubert A. (2014). *Micromorphic approach to crystal plasticity and phase transformation.* In : Plasticity and beyond, eds. Schroeder J. and Hackl K., pp 131–198. CISM International Centre for Mechanical Sciences, Courses and Lectures No. 550, Springer.

Fratzl P., Penrose O., and Lebowitz J.L. (1999). *Modeling of phase separation in alloys with coherent elastic misfit.* Journal of Statistical Physics, vol. 95, pp 1429–1503.

Fried E. and Gurtin M.E. (1993). *Continuum theory of thermally induced phase transitions based on an order parameter.* Physica D, vol. 68, pp 326–343.

Gaubert A., Finel A., Le Bouar Y., and Boussinot G. (2008). *Viscoplastic phase field modellling of rafting in Ni base superalloys.* In : Continuum Models and Discrete Systems CMDS11, eds. Jeulin D. and Forest S., pp 161–166. Mines Paris Les Presses.

Gaubert A., Le Bouar Y., and Finel A. (2010). *Coupling phase field and viscoplasticity to study rafting in Ni-based superalloys.* Philosophical Magazine, vol. 90, pp 375–404.

Gurtin M.E. (1996). *Generalized Ginzburg–Landau and Cahn–Hilliard equations based on a microforce balance.* Physica D, vol. 92, pp 178–192.

Khachaturyan A.G. (1983). *Theory of structural transformations in solids.* John Wiley & Sons.

Kiefer B., Furlan T., and Mosler J. (2017). *A numerical convergence study regarding homogenization assumptions in phase field modeling.* International Journal for Numerical Methods in Engineering, vol. 112, pp 1097–1128.

Kobayashi R., Warren J. A., and Carter W. C. (2000). *A continuum model of grain boundaries.* Physica D, vol. 140 n° 1-2, pp 141–150.

Larché F and Cahn J.W (1973). *A linear theory of thermochemical equilibrium of solids under stress.* Acta Metallurgica, vol. 21, pp 1051–1063.

Larché F. and Cahn J. W. (1978). *A nonlinear theory of thermochemical equilibrium of solids under stress.* Acta Metallurgica, vol. 26, pp 53–60.

Lindroos M., Pinomaa T., Ammar K., Laukkanen A., Provatas N., and Forest S. (2022). *Dislocation density in cellular rapid solidification using phase field modeling and crystal plasticity.* International Journal of Plasticity, vol. 148, pp 103139.

Maugin G. A. (1999). *The thermomechanics of nonlinear irreversible behaviors.* World Scientific.

Maugin G. A. (2006). *On the thermomechanics of continuous media with diffusion and/or weak nonlocality.* Archives of Applied Mechanics, vol. 75, pp 723–738.

Miehe C. (2011). *A multifield incremental variational framework for gradient type standard dissipative solids.* Journal of the Mechanics and Physics of Solids, vol. 59, pp 898–923.

Mosler J., Shchyglo O., and Montazer Hojjat H. (2014). *A novel homogenization method for phase field approaches based on partial rank-one relaxation.* Journal of the Mechanics and Physics of Solids, vol. 68, pp 251–266.

Müller I. (1985). *Thermodynamics.* Pitman Publishing Limited, London.

Pinomaa T., Lindroos M., Jreidini P., Haapalehto M., Ammar K., Wang L., Forest S., Provatas N., and Laukkanen A. (2022). *Multiscale analysis of crystalline defect formation in rapid solidification of pure aluminium and aluminium-copper alloys.* Phil. Trans. R. Soc. A, vol. 380, pp 20200319.

Rancourt V. de, Appolaire B., Forest S., and Ammar K. (2016). *Homogenization of viscoplastic constitutive laws within a phase field approach.* Journal of the Mechanics and Physics of Solids, vol. 88, pp 35–48.

Schmidt S. D., Ammar K., Dornisch W., Forest S., and Müller R. (2021). *Phase field model for the martensitic transformation : comparison of the Voigt/Taylor and Khachaturyan approach.* Continuum Mechanics and Thermodynamics, vol. 33, pp 2075–2094.

Steinbach I. (2009). *Phase field models in materials science.* Modelling and Simulation in Materials Science and Engineering, vol. 17, pp 1–31.

Steinbach I. and Apel M. (2006). *Multi phase field model for solid state transformation with elastic strain.* Physica D, vol. 217, pp 153–160.

Steinbach I. and Shchyglo O. (2011). *Phase-field modelling of microstructure evolution in solids : Perspectives and challenges.* Current Opinion in Solid State and Materials Science, vol. 15, pp 87–92.

Ubachs R.L.J.M., Schreurs P.J.G., and Geers M.G.D. (2004). *A nonlocal diffuse interface model for microstructure evolution of tin–lead solder.* Journal of the Mechanics and Physics of Solids, vol. 52, pp 1763–1792.

Ubachs R.L.J.M., Schreurs P.J.G., and Geers M.G.D. (2005). *Phase field dependent viscoplastic behaviour of solder alloys.* International Journal of Solids and Structures, vol. 42, pp 2533–2558.

Ubachs R.L.J.M., Schreurs P.J.G., and Geers M.G.D. (2006). *Microstructure dependent viscoplastic damage modelling of tinlead solder.* Journal of the Mechanics and Physics of Solids, vol. 54, pp 2621–2651.

Ubachs R.L.J.M., Schreurs P.J.G., and Geers M.G.D. (2007). *Elasto-viscoplastic nonlocal damage modelling of thermal fatigue in anisotropic lead-free solder.* Mechanics of Materials, vol. 39, pp 685–701.

Villani A., Busso E.P., Ammar K., Forest S., and Geers M.G.D. (2014). *A fully coupled diffusional-mechanical formulation : numerical implementation, analytical validation, and effects of plasticity on equilibrium.* Archive of Applied Mechanics, vol. 84, pp 1647–1664.

Wang Y. and Khachaturyan A.G. (1995). *Shape instability during precipitate growth in coherent solids.* Acta Metall. mater., vol. 43 n° 5, pp 1837–1857.

Wang Y., Khachaturyan A.G., and Morris J.W. Jr (1993). *Kinetics of strain-induced morphological transformation in cubic alloys with a miscibility gap.* Acta metall. mater., vol. 41, pp 279–296.

Warren J. A., Kobayashi R., Lobkovsky A. E., and Carter W.C. (2003). *Extending phase field models of solidification to polycrystalline materials.* Acta Materialia, vol. 51, pp 6035–6058.