Tytuł: Stochastyczny model rozwoju mikrostruktury i własności metali poddawanych obróbce cieplnomechanicznej

Title: Stochastic approach to modelling microstructure evolution and properties of metals subjected to thermomechanical processing

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Research team

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Motivation.

Continuous development of transport, including airplane, automotive, and rail industries, is associated with the search for new construction materials that combine high strength with good plastic properties. Steels meet these high requirements and due to their low costs of manufacturing and good recyclability they are still commonly used in the transportation industry. Intensive research during last few decades have shown that there is still a huge potential for improvements of properties of steels. Objectives of research on steels were focused on an increase of strength while maintaining good workability. Multiphase microstructures allow to obtain high strength but, contradictory, relatively smooth gradients of properties are needed to obtain good local fracture resistance. Advanced numerical models are needed to gain knowledge on distributions of microstructural features and to design thermal-mechanical cycles allowing to obtain moderate gradients of properties. A hypothesis was made that description of the heterogeneous microstructure of multiphase steels with the distribution functions of various microstructure features, will allow to build the model with capability to predict gradients of final product properties.

Objectives and scientific problem aimed to be solved

To prove the main hypothesis of the project the general objective was proposed as development of the distribution functions describing such features of microstructure as elements distribution in different phases, dislocation density, grain size and morphology, and size of precipitates. Adaptation of existing microstructure evolution and phase transformation models to stochastic independent variables is one of the aims.

The main objective of the project is solution of differential equations describing evolution of materials microstructure for stochastic variables. Such a solution is possible using numerical methods (eg. Monte Carlo). These methods are computationally expensive and prove of the existence and uniqueness of the solution is problematic. Therefore, particular objectives of the project are focused on exploring possibilities of analytical solution of differential evolution equations.

Since proposed solutions are computationally expensive, simplification of the computational domain is the next objective. RVE is substituted by the Statistically Similar Representative Volume Element (SSRVE).

The global scientific goal of the project is focused on expanding computational capabilities in material modelling, in order to predict advanced microstructure parameters and material properties. In consequence, an efficient tool for the design of manufacturing of new generation multiphase materials will be created.

Significance and pioneering nature of the project

As it has been mentioned, multiphase steels meet high requirements and are still commonly used in the transportation industry. These steel grades are characterised by heterogeneous multiphase microstructures and require very complex thermo-mechanical treatment processes and precise control of technological parameters. Design of these processes can be noticeably improved by numerical models, which combine prediction of thermal-mechanical cycles resulting in required microstructure with modelling of microstructure evolution and phase transformations occurring during these cycles. Modelling of micro scale phenomena (microstructure evolution and phase transformations) is now commonly based on either mean field or advanced multiscale models. The former are fast but they do not supply information on the gradients

of properties, which is crucial for the design of new steels. The latter are capable to predict distribution functions but they involve very long computing times and cannot be used in design process, which is based on optimization procedures. Realization of the project will supply the model, which combines extensive predictive capabilities of the RVE models with low computing costs of the mean field models. In consequence, the model will be an efficient tool supporting design of processes for advanced steels. Although all numerical tests in the project will be performed for multiphase steels, the model will be general and can be directly used to any heterogeneous material, whose evolution is described by differential equations.

Research

As a step in description of the evolution of statistical properties of the model we have started with simplified differential equations similar in nature to the original one [1]. Our aim was to find mathematically strict, analytic formula for their solutions. A mathematical background, analysis various approximations of the solution and proof of its stability is presented in [3]. This was a testing ground for different numerical methods (discretization), when searching for the most accurate method. After choice of the most promising numerical methods we have found (numerical) descriptions of the evolution of distributions of parameters of the material, when these parameters change in time as an effect of applied metal forming. In parallel the statistically similar representative volume element was design to reduce computing times [2]. Computing costs were compared in the review of mean field and full field models [4] and sensitivity analysis as well as validation of the model is described in [5]. Following this, the inverse problem was formulated [6]. When knowing the desired distribution of the solution, one would be able to back-calculate the required parameters. The obtained results will be compared with the experimental data from the partners in other projects.

Publications

- 1. Morkisz P., Oprocha P., Przybyłowicz P., Czyżewska N., Kusiak J., Szeliga D., Rauch Ł., Pietrzyk M., prediction of distribution of microstructural parameters in metallic materials described by differential equations with recrystallization term, International Journal for Multiscale Computational Engineering, 17(3), 2019, 361–371.
- 2. Ł. Rauch, K. Bzowski, D. Szeliga, M. Pietrzyk, Development and application of the Statistically Similar Representative Volume Element for numerical modelling of multiphase materials, in: V. Krzhizhanovskaya et al. (eds), Computational Science ICCS 2020, Lecture Notes in Computer Science, vol 12142. Springer, Cham, 2020, 1-14.
- 3. Czyżewska N., Kusiak J., Morkisz P., Oprocha P., Pietrzyk M., Przybyłowicz P., Rauch Ł., Szeliga D., On mathematical aspects of evolution of dislocation density in metallic materials, Nonlinear Differential Equations and Applications NoDEA, 2020 (submitted).
- 4. D. Szeliga, K. Bzowski, Ł. Rauch, R. Kuziak, M. Pietrzyk, Mean field and full field modelling of microstructure evolution and phase transformations during hot forming and cooling of low carbon steels, Computer Methods in Materials Science, 2020 (in review).
- 5. D. Szeliga, N. Czyżewska, K. Klimczak, J. Kusiak, P. Morkisz, P. Oprocha, M. Pietrzyk, P. Przybyłowicz, Sensitivity analysis, identification and validation of the dislocation density-based model for metallic materials (submitted)
- 6. K. Klimczak, P. Oprocha, J. Kusiak, D. Szeliga P. Morkisz, P. Przybyłowicz, N. Czyżewska, M. Pietrzyk, Inverse problem in stochastic approach to modelling of microstructural parameters in metallic materials during processing, (to be submitted)

Conferences

- 7. N. Czyżewska, J. Kusiak, P. Morkisz, P. Oprocha, M. Pietrzyk, P. Przybyłowicz, Ł. Rauch, D. Szeliga, On mathematical aspects of evolution of dislocation density in metallic materials, Konferencja zastosowań matematyki, Zakopane, 2018.
- 8. D. Bachniak, Ł. Rauch, D. Szeliga, M. Pietrzyk, Stochastic modelling of phase transformations using HPC infrastructure, KUKDM, Zakopane 2018.
- 9. D. Szeliga, Ł. Rauch, M. Pietrzyk, identification of the multiscale material model based on an internal variable, SolMech, Warszawa, 2018.
- 10. P. Morkisz, P. Oprocha, P. Przybyłowicz, N. Czyżewska, J. Kusiak, D. Szeliga, M. Pietrzyk, Prediction of distribution of microstructural parameters in steels described by differential equations with recrystallization term: two possible approaches, WCCM, New York, 2018.
- 11. N. Czyżewska, On mathematical aspects of evolution of dislocation density in metallic materials, Int. Conf. KomPlasTech, Zakopane, 2019.

- 12. N. Czyżewska, Jak wytworzyć stal o oczekiwanych własnościach czyli o nieliniowych równaniach różniczkowych z opóźnieniem oraz o ich numerycznej aproksymacji, Studencka Konferencja Zastosowań Matematyki DwuMIan, Warszawa, 2019.
- 13. N. Czyżewska, Jak wytworzyć stal o nieoczekiwanych własnościach czyli o nieliniowych równaniach różniczkowych z opóźnieniem oraz o ich numerycznej aproksymacji, Ogólnopolska Konferencja Studentów Matematyki "Oblicze", Poznań, 2019.
- 14. N. Czyżewska, pt. "O tym, jak matematyk może pomóc w produkcji lepszej stali, IV Studencka Konferencja "Oblicza współczesnej matematyki" Studenckiego Koła Matematyków AGH, Kraków, 2019.
- 15. N. Czyżewska, Nonlinear delay differential equations and its numerical approximation on an example of steel production, The 8th International Conference on System Modeling and Optimization ICSMO, Barcelona, 2020.
- 16. D. Szeliga, Ł. Sztangret, K. Klimczak, J. Kusiak, M. Pietrzyk, Identification of the multiscale material model based on a stochastic internal variable, Conf. ADMOS, Alicante, 2019.
- 17. N. Czyżewska, On mathematical aspects of evolution of dislocation density in metallic materials, ECCOMAS Young Investigators Conference YIC, Kraków, 2019..
- 18. Rauch, K. Bzowski, K. Czechowicz, D. Szeliga, M. Pietrzyk, Set up of the RVE for properties simulation in multiphase steels, Proc. Conf. MEFORM, Freiberg, 2020, 59-64.