Microstructure simulation techniques for accelerating the development process of structural materials

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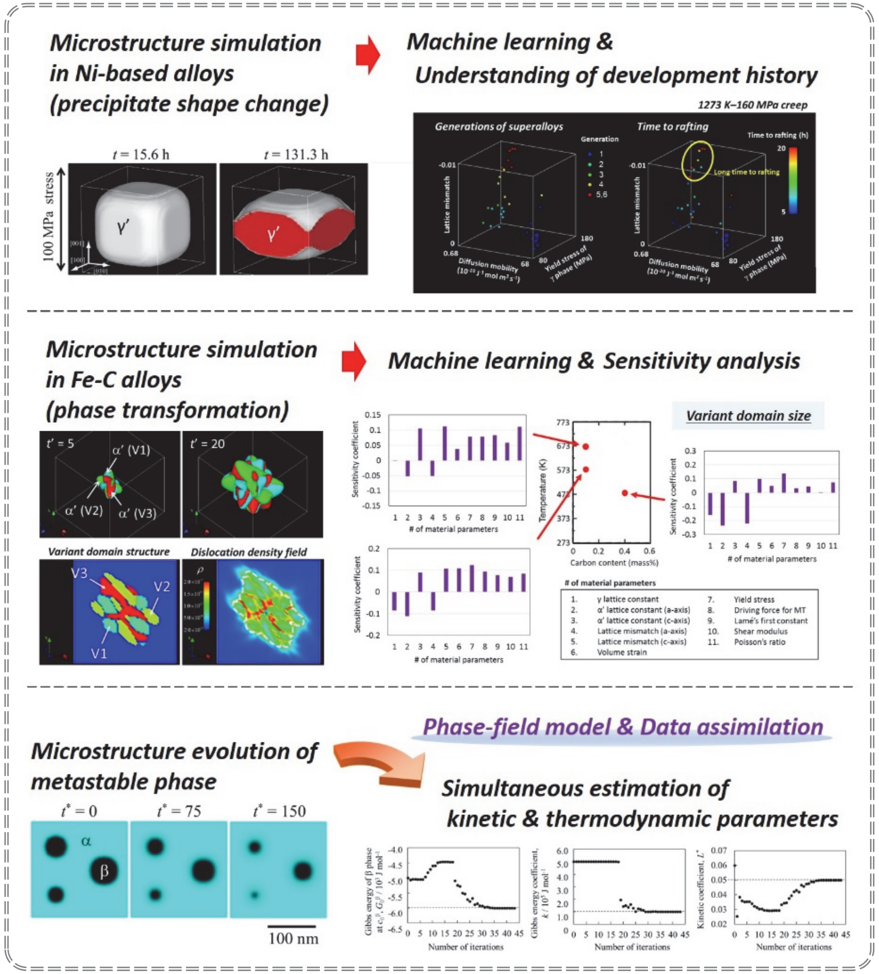
Research Area ：Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

Brief overview

Microstructure control is important for improving material properties. In this study, microstructure evolution in structural materials is modeled on the basis of the phase-field (PF) method. Simulations are performed under various conditions of material parameters in the PF models. The obtained data are used for machine learning to enable fast predictions of microstructure and elucidate effects of material parameters on microstructure characteristics. On the other hand, we propose a method for estimating/optimizing material parameters involved in a PF model from experimental data on microstructure evolution.



Achievement

We enabled fast predictions of precipitate shape change during creep in nickel-based alloys and microstructure evolution during martensitic transformation in steels. We have shown that (i) the generation of nickel-based alloys is closely related to the rate of precipitate shape change during short-term creep and (ii) sensitivities of material parameters to martensite microstructure in steels differ depending on the conditions of temperature and composition. On the other hand, we have shown that Gibbs energy of a metastable phase can be estimated from experimental data on microstructure by a data assimilation technique.

Reference/Link

- Y. Tsukada, T. Koyama, F. Kubota, Y. Murata, Y. Kondo, Intermetallics 85 (2017) 187-196.
- Y. Tsukada, E. Harata, T. Koyama, Proc. of the 5th International Symposium on Steel Science, pp. 127-130, 2017.
- http://www.material.nagoya-u.ac.jp/PFM/

As for related strategic objectives related to this research area, see http://www.senryaku.jst.go.jp/teian/en/koubo/h29youkou_7_en.pdf