

Large scale simulations of solidification and grain growth at atomistic and microstructural scales

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In the making process of structural materials, there are many types of phase transformation, which leads to a variety of microstructure. Therefore, it is desired to understand the microstructure formation process and control them with a high degree of accuracy. Especially, it is not straightforward to observe and analyze solidification and subsequent grain growth from the experimental approach. Hence, it is strongly desired to reveal them from the computational approach. We have investigated microstructure formation from the dynamic point of view by way of large-scale simulations including molecular dynamics (MD) and phase-field method (PFM). Particularly, the estimation of physical properties of microstructure [1] and the atomistic detail of solidification and grain growth by MD simulation [2], the development of high-accuracy phase-field model for large-scale simulation [3], and the dendritic growth and grain growth in polycrystalline microstructure by PFM [4] are main achievements of our study. In the presentation, our cutting-edge results are introduced, and present and future of researches of materials process based on large-scale simulation will be discussed.

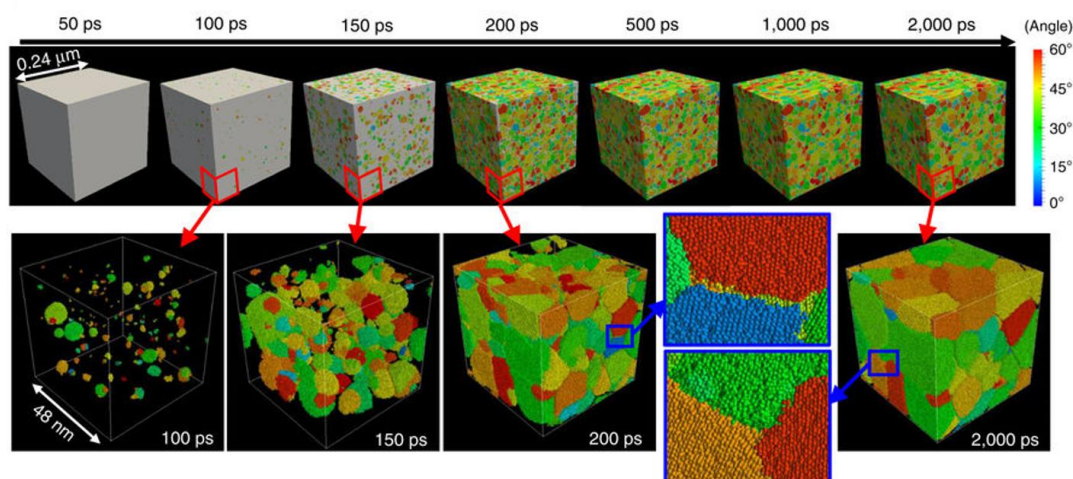


Figure. 1 Very large scale molecular dynamics simulation of homogenous nucleation and solidification from undercooled melt iron. (1,040,000,000 atoms) [1]

Bibliography

- [1] S.K. Deb Nath, Y. Shibuta, M. Ohno, T. Takaki, T. Mohri; ISIJ Int. **57**, 1774 (2017).
- [2] Y. Shibuta, et al.; Nature Communications, **8**, 10 (2017)
- [3] M. Ohno, T. Takaki, Y. Shibuta; Phys. Rev. E, **96**, 033311 (2017).
- [4] E. Miyoshi et al; npj Computational Materials, **3**, 25 (2017).

External links

<http://www.mse.t.u-tokyo.ac.jp/> (Materials Modelling Lab, The University of Tokyo)

<http://www.cmd.kit.ac.jp/> (Computational Materials Design Lab, Kyoto Institute of Technology)