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Molecular dynamics study of dual-phase microstructure of Titanium and Zirconium metals during the quenching process NARUMASA MIYAZAKI, KAZUNORI SATO, YOJI SHIBUTANI, Osaka University — Dual-phase (DP) transformation, which is composed of felite- and/or martensite- multicomponent microstructural phases, is one of the most effective tools to product functional alloys. To obtain this DP structure such as DP steels and other materials, we usually apply thermal processes such as quenching, tempering and annealing. As the transformation dynamics of DP microstructure depends on conditions of temperature, annealing time, and quenching rate, physical properties of materials are able to be tuned by controlling microstructure type, size, their interfaces and so on. In this study, to understand the behavior of DP transformation and to control physical properties of materials by tuning DP microstructures, we analyze the atomistic dynamics of DP transformation during the quenching process and the detail of DP microstructures by using the molecular dynamics simulations. As target metals of DP transformation, we focus on group 4 transition metals, such as Ti and Zr described by EAM interatomic potentials. For Ti and Zr models we perform molecular dynamics simulations by assuming melt-quenching process from 3000 K to 0 K under the isothermal–isobaric ensemble. During the process for each material, we observe liquid to HCP like transition around the melting temperature, and continuously HCP-BCC like transition around martensitic transformation temperature. Furthermore, we clearly distinguish DP microstructure for each quenched model.

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