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Application of multi-scale modeling to deformation of Metal under uniaxial tension

OGAWA, Takaki, LIU, Hebin and NAKATANI, Akihiro

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SUMMARY

Recently the importance of multi-scale analysis is increasing. For the multi-scale analysis there are three key points; the definition of value of concern, the decision of tratement scale, and the concideration of computational costs.

Kevrekidsis et al. present equation-free (EF) method for computer-aided multiscale analysis. The method enables models at a microscopic level of description to perform modeling tasks at a macroscopic level. This method is a framework to analyze macro value evolution using only micro time and micro space in the micro simulation, without the governing equations on the macro scale field. If we are able to adapt this framework to the structural analysis by using finite element method (FEM) which has been widely used in the industrial sector, we can analyze with reducing the freedom of the system. Therefore, this framework has the potential of an effective technique to the analysis for further large-scale structure, etc.

The purpose of this study is to apply a multi-scale modeling approach using equation-free method to the problem for solid mechanics.

First, we consider cubic single crystal structure face-centered cubic (fcc) Cu consisting of 38,880. Molecular dynamics (MD) simulations are carried out to this model under uniaxial tension. Next, we carry out continuum approach for the same scale model and consider the difference between the continuum mechanics approach. In this case, we use the general-purpose finite element method structural analysis solver LS-DYNA for the macro simulation. Finally, we code equation-free method for the LS-DYNA subroutine and discuss the possibility of application this framework with the coupling MD and FEM for the problem of solid mechanics.