

Supplementary information for

Homogeneous nucleation and microstructure evolution in million-atom molecular dynamics simulation

Yasushi Shibuta^{1*}, Kanae Oguchi¹, Tomohiro Takaki² and Munekazu Ohno³

¹Department of Materials Engineering, The University of Tokyo

7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

²Mechanical and System Engineering, Kyoto Institute of Technology

Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan

³Division of Materials Science and Engineering, Faculty of Engineering, Hokkaido University

Kita 13 Nishi 8, Kita-ku, Sapporo, Hokkaido 060-8628, Japan

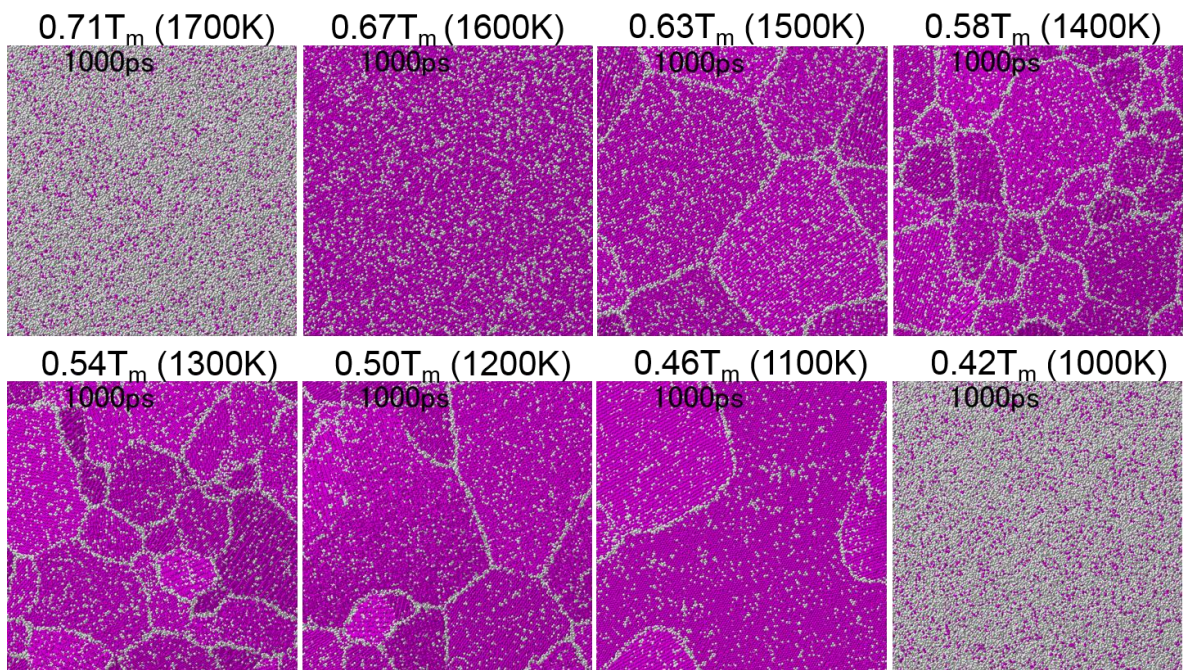


Figure S1. (a) Snapshots of the representative atomic configuration after 1000 ps calculation for each temperature.

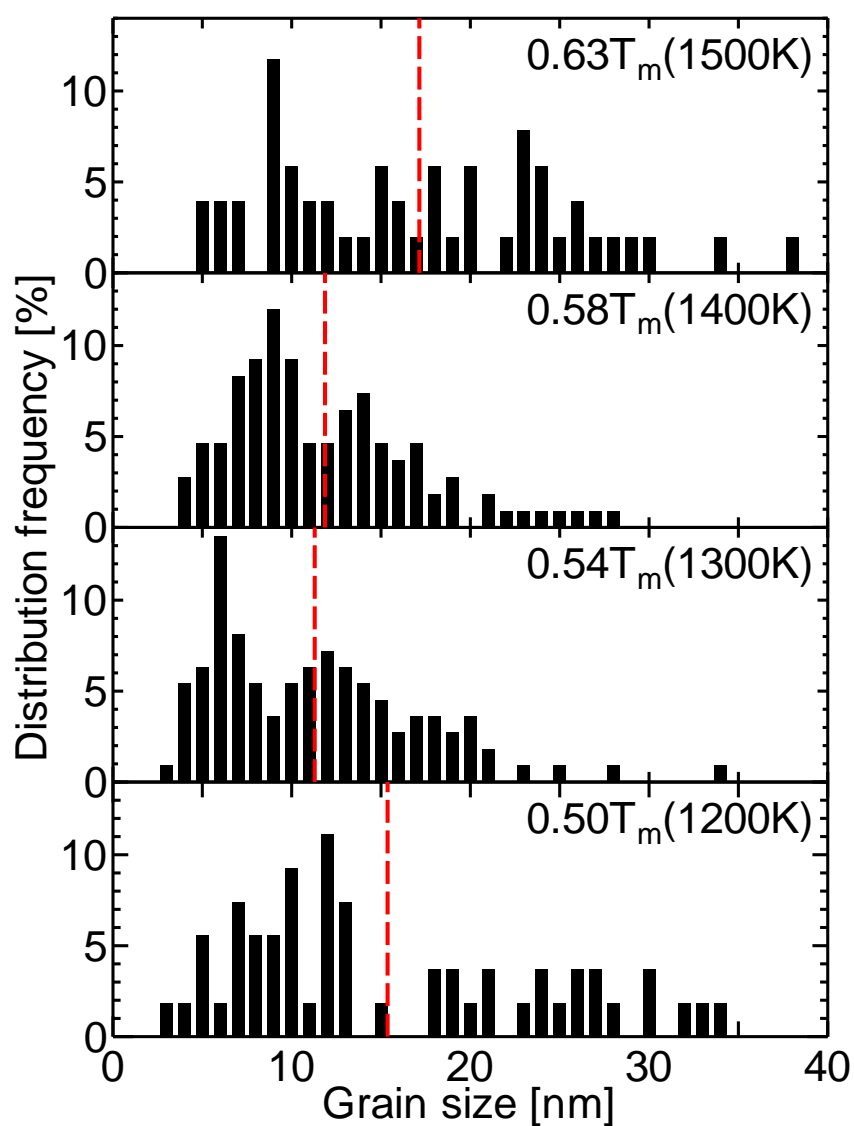


Figure S2. Grain size distribution directly measured from the snapshots at 1000 ps from five replicate calculations for each temperature. The grain size distribution is normalized by total grain number for each temperature. Red dashed lines represent the arithmetic average of the grain size.