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Effect of Mg^{2+} on the structure of amorphous $CaCO_3$ – A molecular dynamics simulation HIDEKAZU TOMONO, HIROKI NADA, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, JAPAN — Molecular dynamics (MD) simulations of amorphous calcium carbonate (ACC) were carried out to investigate the effect of Mg^{2+} ions on the structure of $CaCO_3$ crystal nucleus formed from ACC. Our systems contained 432 $CaCO_3$ with several concentrations of $MgCO_3$. In this study, our original ion model of Mg^{2+} was developed and combined with Raiteri model of Ca^{2+} and rigid ${CO_3}^{2-}$ [1]. The simulations indicated that the fraction of vaterite-like ion arrangement was much larger than those of calcite-like and aragonite-like ion arrangements in pure ACC. However, as the Mg^{2+} concentration increased, the faction of vaterite-like ion arrangements decreased, which suggests that Mg^{2+} ions play as inhibitors of vaterite nucleation. The result explains why calcite or aragonite is preferentially nucleated in the presence of Mg^{2+}, whereas vaterite is nucleated in the absence of them.[1] P. Raiteri, J. D. Gale, D. Quigley, and P. M. Rodger, J. Phys. Chem. C 114, 5997 (2010).

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