

Abstract Submitted  
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**Structural evolution of Mg and Mg-rich bulk alloy during thermal expansion and rapid quenching by ab initio molecular dynamics** MASAE TAKAHASHI, IMR, Tohoku University — Magnesium alloy are becoming more and more attractive for lightweight structural application. Recently, the Mg bulk alloy containing a very small amount of Zn and Y with excellent mechanical properties was developed. To reveal the wonderful effect of the very small amount of additives and furthermore evidence our recent prediction of anisotropic elongation in c-axis in the inflation process of Mg-clusters under charge transfer in bulk alloy, we investigated here structural transitions of Mg and Mg-rich alloy during thermal expansion and quenching processes by ab initio molecular dynamics simulation. The variations with temperature of linear thermal expansion coefficients, total energies, and radial distribution functions have been characterized. Anisotropic thermal expansion of Mg metal and the discrete jump of thermal expansion coefficients around 700 K was found. During the expansion processes, simple thermal vibrations, large atomic displacements in ab plane, and additional displacements in the direction of c axis were observed. The results qualitatively agreed with experimental observation.

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