ABSTRACT
The materials properties are strongly related to their microstructure, which is affected their processing. It is difficult for first-principles calculations to apply directly to materials design because the scale of the calculations is only about a hundred atoms. However, the first-principles calculations can approach to mechanism of materials properties using suitable modeling based on experimental results. The first-principles study of Mg–Zn–Ca alloys exhibiting high-stretch formability is an example. It is demonstrated experimentally that Mg–Zn–Ca alloy sheets show high-stretch formability although Mg–Zn and Mg–Ca alloy sheets do not show such formability. The calculation study focuses on improved plastic anisotropy of Mg–Zn–Ca alloys, and the improved plastic anisotropy gives rise to the reduced basal plane texture, resulting in the high formability of Mg–Zn–Ca alloys.
projects is evaluation of the highly formable Mg alloys, which are developed in his research group. He also interested in twinning of Mg.