Usage Report for Fiscal Year 2018

Project Title:

Computational Discovery of novel ternary borides

Name: Mohammad Khazaei
Laboratory at RIKEN: Computational Materials Science Research Team, RIKEN Center for Computational Science, Kobe

1. Background and purpose of the project, relationship of the project with other projects

Chemical exfoliations of layered materials has opened a way to synthesis novel two-dimensional (2D) materials. In this regard, layered boride phases, known as MAB phases are considered as a great source for obtaining 2D transition metal borides. MAB phases are orthorhombic crystals with chemical formula of MAB, M_2AB_2, $M_3A_2B_2$, M_3AB_4, and M_4AB_6. Currently, MAB phases possess few members: MoAlB, WAlB, Cr_2AlB_2, Mn_2AlB_2, Fe_2AlB_2, Cr_3AlB_4, and Cr_4AlB_6. In this project, I have examined the possibility to extend the family of MAB phases to other transition metals such as M = Sc, Ti, Zr, Hf, V, Nb, Ta, Tc, Ru, Ru, Co, Rh, Ir, and Ni.

2. Specific usage status of the system and calculation method

At first, I have collected all possible crystal structures of M-Al and M-B binary and M-Al-B ternary compounds using Springer Crystal Structure Data base. By using first-principle density functional theory, I have calculated the formation energy (ΔH) formation of MAB phases with respect to combinations of most competitive phases; $\Delta H = E_{tot}(\text{MAB phase}) - E_{tot}(\text{competitive phases})$, where E_{tot} is the total energy.

3. Result

In order to observe the trend better, the ΔH is plotted with respect to transition metals in Figure 1. The negative (positive) ΔH indicates the relative stability (instability) of MAB phases with respect to the competitive phases. The more negative (positive) ΔH indicates the higher (smaller) chance for synthesis of the MAB phases experimentally. In excellent agreement with experimental observation, some of the Cr-, Mo-, W-, Mn-, and Fe-based MAB phases find negative ΔH, indicating their synthesis possibility in experiment. The negative DH of Tc-based MAB phases implies the high chance for their synthesis although there has been no experimental report. This might be due to the lack of experiments on Tc-based MAB phases or there might be some binary Tc-Al or Tc-B, or ternary Tc-Al-B phases that have not been characterized experimentally yet, preventing the formation of Tc-based MAB phases. Further experiments on Tc-Al-B are highly desirable for discovery of new Tc-Al, Tc-B, or Tc-Al-B phases.

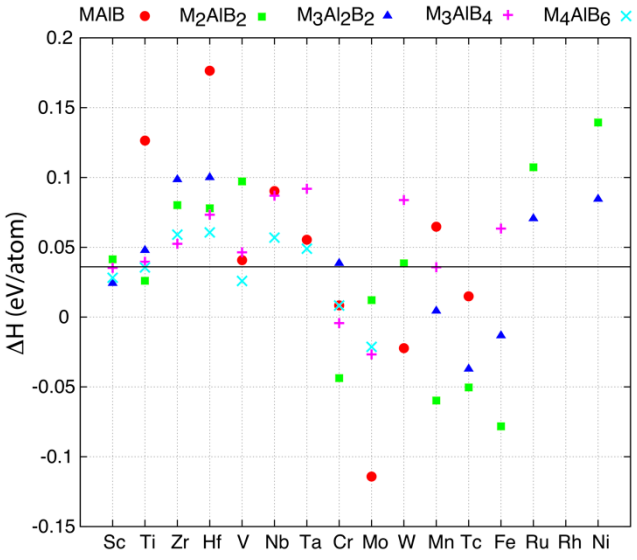

Figure 1. The relative formation energy DH of various MAB phases. The solid black line indicates ΔH = 0.036 eV/atom.

According to the recent computational screening on inorganic crystal structure data base (ICSD), 20% of all compounds have instability of ΔH larger than 0.036 eV/atom. Assuming this value as a stability

criterion (i.e., $\Delta H < 0.036$ eV/atom), it is expected that there is a possibility for experimental synthesis of Sc-, Ti-, and V-based MAB phases, in addition to Cr-, Mo-, W-, Mn-, Tc-, Fe-, and Ru-based MAB phases.

4. Conclusion

By comparing the formation energies of these MAB phases with those of their available competing binary M-B and M-Al, and ternary M-Al-B phases, we find that some of the Sc-, Ti-, V-, Cr-, Mo-, W-, Mn-, Tc-, and Fe-based MAB phases can be favorably synthesized in an appropriate experimental condition.

5. Schedule and prospect for the future

In this study, I investigated the formation possibility of Al-containing MAB phases. In the future, I would like to extend it to other A elements such as Si, Ga, Ge, P, As, and S.