First Principles Calculations of Superconducting Transition Temperature of $ThCr_2Si_2$-type Structure

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High superconducting transition temperature (T_c) superconductors have a great potential in many industrial applications. However, discovering a compound having high T_c is still remaining a big challenge for experimental approach due to time-consuming and high cost. In this talk, we focus on $ThCr_2Si_2$-type compounds with a *I*4/*mmm* symmetry (Fig.1(a),(b)) and predict their T_c values by combining first-principles phonon simulations with models based on the Bardeen-Cooper-Schrieffer (BCS) theory [1]. Although thousand compounds belong to this structure, no comprehensive and systematic study has been done so far. Referring to the NIMS database [2], our T_c results showed a fairly good agreement with the experimental data (Fig.1(c)). Finally, our exploration within the $ThCr_2Si_2$ family revealed that $ThCu_2Si_2$ and $ThAu_2Si_2$ could be newly possible conventional superconductors having T_c around 3.88 K and 4.27 K, respectively [3]. Here our first principles phonon simulations confirmed that both of compounds have non-negative frequencies indicating the dynamical stability of the compounds at ambient temperature. In addition, we found that Fe or Co based compounds could not be explained just by electron-phonon interaction. This discrepancy between theory and experiment implies that those compounds are unconventional superconductors.

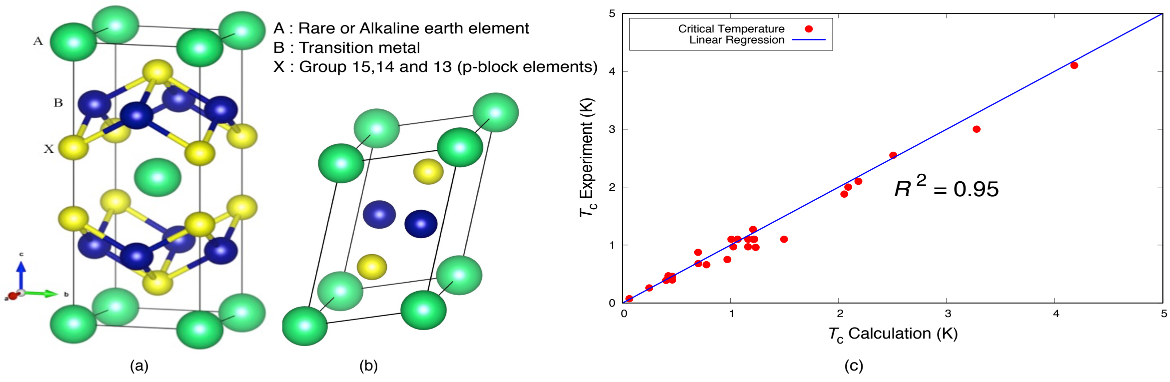

Fig 1. (a) The conventional unit cell of AB_2X_2 with tetragonal $ThCr_2Si_2$-type structure and (b) primitive cell. (c) comparison calculated T_c based on BCS theory and experiment results for conventional superconductors showed a fairly good agreement with *R*-squared = 0.95.

[1] K. Nakano, K. Hongo, and R. Maezono, Sci. Rep. 6, 29661 (2016).

[2] "Superconducting material database (supercon)," https://supercon.nims.go.jp/supercon/material_search, accessed: 2019-11-17

[3] G.S Sinaga, K. Uchimura, K. Nakano, K. Hongo, and R. Maezono, arXiv:1911.10716