(6b1)

Raman Scattering of skutterudite compounds

N. Ogita[1], M. Udagawa[1], T. Kondo[2], C. Sekine[3], I. Shirotani[3], H. Sugawara[4], Y. Aoki[5], and H. Sato[5]

[1]Faculty of Integrated Arts & Sciences, Hiroshima Univ., Higashi-Hiroshima 739-8521
[2]Venture Business Laboratory, Hiroshima Univ., Higashi-Hiroshima 739-8527
[3]Faculty of Engineering, Muroran Institute of Technology, Muroran, 050-8585
[4]Faculty of Integrated Arts and Sciences, Tokushima Univ., Tokushima 770-8502
[5]Department of Physics, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397

Raman scattering spectra of the filled skutterudite RT_4X_{12} (R=La, Ce, Pr and Nd, T=Fe, Os, X=P, Sb) and the unfilled CoP_3 have been measured. In the skutterudite family with cubic symmetry of $Im\bar{3}$ (T_h^5), Raman active mode is $2Ag + 2Eg + 4Tg$. All Raman active modes are the vibrations of pnictogens; P or Sb.

To clarify the lattice dynamics of the skutterudite compounds, normal mode analysis has been made, by means of a GF matrix method. In this analysis, we employed seven force constants, that is, longitudinal atomic-interactions due to the shortest seven bond length as shown in left panel of figure 1. Seven force constants have been determined by optimizing the difference between the observed energies of the eight Raman active phonons and the calculated ones.

The most characteristic result is a strong force constants between rare-earth ion and surrounding atoms. The bond-length dependence of this force constant is shown in right panel of figure 1, where this kinds of the force constants in the other rare-earth compounds are also plotted, such as Kondo compounds of CeNiSn and CeRhSb, and hexaborides. The result shows the existence of p-f hybridization in the skutterudite compounds. Especially, the fraction due to the hybridization becomes larger for the ROs_4Sb_{12}.

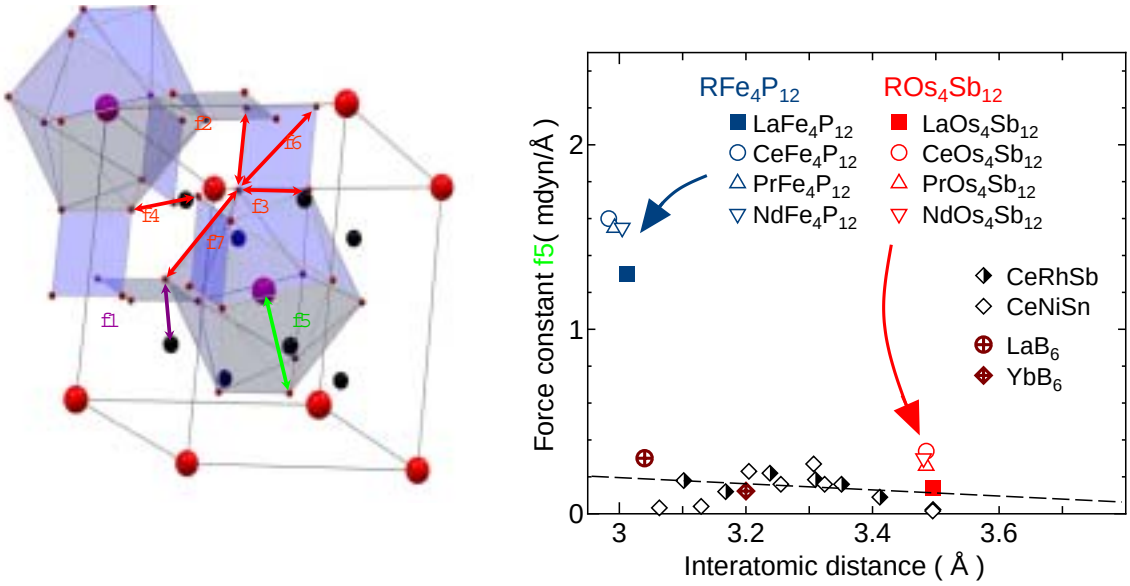

Figure 1: a)left panel: employed seven force constants in this normal mode analysis. b)right panel: Bond-length dependence of force constant between rare-earth and surrounding ions.