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Study of rattling mechanism by thermal factor analyses of EXAFS

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Extended X-ray absorption fine structure (EXAFS) measurements have been carried out on $\text{ROs}_4\text{Sb}_{12}$ ($\text{R}=\text{La}, \text{Ce}, \text{Pr}, \text{Nd}, \text{Sm}$) at BL9A and BL12C with Si(111) monochromator at Photon Factory (KEK) to study the motion of rare earth ions accommodated in Sb icosahedron cage. Temperature dependences of the thermal (Debye-Waller) factors were analyzed from 15 to 300K. In this study, Einstein model was applied to analyze thermal factor. Figure 1(a) shows Einstein temperature obtained from EXAFS and the energy of the second order phonons from raman scattering measurement¹⁾. The absolute values of them are different each other, but the cage space(the space inside Sb icosahedron cage) dependence of these compounds is same. On the other hand, the local static disorder obtained from the temperature dependence of EXAFS has a good correlation with cage space for various rare earth ions. The static distortion is expected to appear when the cage space is larger than about 0.5\AA .

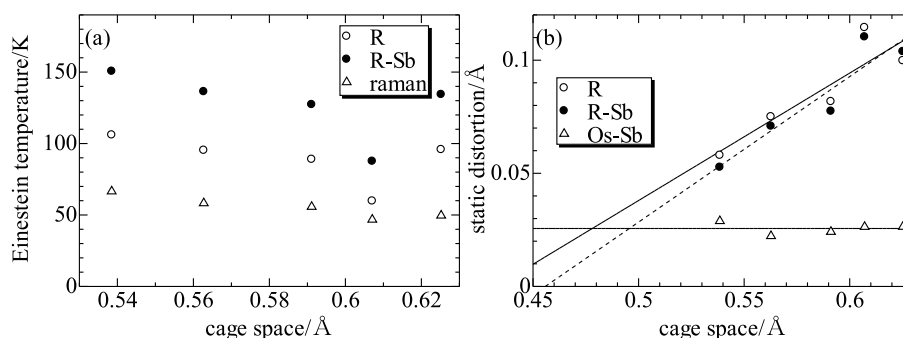


Figure 1: (a) Einstein temperature of R(open circle) and R-Sb(close circle) oscillator as a function of the cage space for $\text{ROs}_4\text{Sb}_{12}$. R: La, Ce, Pr, Nd and Sm. The energy of the second order phonons measured by raman scattering¹⁾(open triangle) is also shown. (b) Static distortion of R(open circle) R-Sb (close circle) and Os-Sb (open triangle) oscillator as a function of the cage space for $\text{ROs}_4\text{Sb}_{12}$. R: La, Ce, Pr, Nd and Sm. Solid and dashed straight line shows linear fit of data.

¹⁾N. Ogita, R. Kojima, Y. Takasu, T. Hasegawa, T. Kondo, M. Udagawa, N. Takeda, T. Ikeno, K. Ishikawa, H. Sugawara, D. Kikuchi, H. Sato, C. Sekine and Y. Shirotani: J. Magn. Magn. Mate. **310** (2007) 948.