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Elastic anomalies due to band electrons in skutterudite compounds

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Filled skutterudite compounds show various interesting properties. In particular, orbital degree of freedom plays a relevant role in Pr-based systems. Large elastic softening, which was found in some compounds, has been considered to be caused by non-Kramers Γ_{23} ground state. On the other hand, it is thought that a particular band nature such as nesting causes M-I transition in $PrRu_4P_{12}$ [1]. The band nesting is expected to associate elastic anomaly.

We have investigated the contribution of band electrons to the elastic constants in filled skutterudite compounds. Together with symmetry consideration, we tried to evaluate the elastic anomalies based on the real band scheme. It has been pointed out that the electronic bands near Fermi energy are approximated by tight binding manner [2]. We assumed the first, second and third nearest neighbor transfer integrals between rare earth atoms in BCC crystal, and then got the band parameters by comparing to the band calculation by Harima $et\ al$ [1]. This method, which resembles casting process of iron, provides us with a method for easy calculation of various physical properties.

Figure 1 shows the temperature dependence of the elastic constants $(C_{11}-C_{12})/2$ and C_{44}. A large elastic anomaly in $(C_{11}-C_{12})/2$ is due to the band nesting. $PrRu_4P_{12}$ shows M-I transition at 60 K. Below this temperature, the elastic constants increase, which is accompanied with the decrease of carrier density [3]. The electron-phonon coupling constant can be evaluated to be 820 K and 1450 K for $(C_{11}-C_{12})/2$ and C_{44}, respectively. The smaller anomaly of $(C_{11}-C_{12})/2$ for $PrFe_4P_{12}$ indicates relatively poor nesting compared to $PrRu_4P_{12}$.
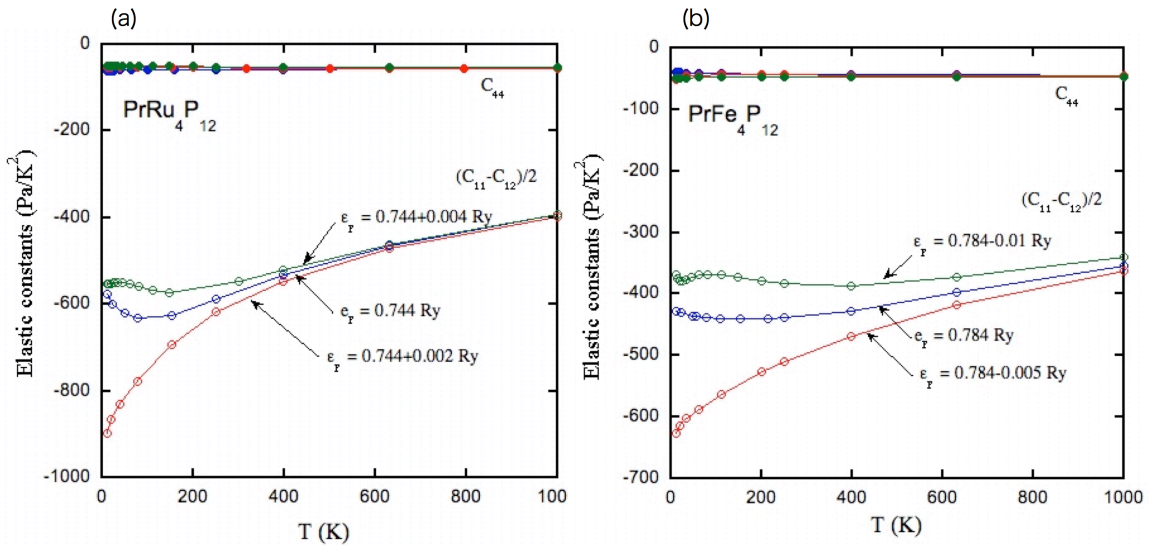

Figure 1: Calcuted elastic constants $(C_{11} - C_{12})/2$ and C_{44} as a function temperature for the cases of (a) $PrRu_4P_{12}$ and (b) $PrFe_4P_{12}$.

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