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**Ce γ→α Phase Transition : The Role of Lattice**

I.-K. Jeong, T.W. Darling, M.J. Graf, Th. Proffen, R.H. Heffner (Los Alamos National Lab.), Y. Lee, and T. Vogt (BNL)

Beamline(s): X7A

**Introduction**: The γ→α phase transition of Ce has been a subject of scientific interests for a long time due to its unusual properties at the transition. It accompanies huge volume collapse (~17%) at the transition. In addition, despite this large volume contraction, the γ→α phase transition is known to be iso-structural (fcc) from a high volume γ-phase to a low volume α-phase as a function of temperature and pressure. At 300K the phase transition occurs around 0.77 GPa.

The γ→α phase transition has been described as a transition driven by an instability of 4*f* electrons in a number of theoretical models including a promotional model, Mott transition and Kondo-volume-collapse models. In these models, therefore, the proper description of the nature of 4*f* electrons in γ- and α-phase has been a key issue. On the contrary, despite the large volume collapse and the unusual elastic properties near the transition, the role of lattice in the transition has received almost no attention.

Recent studies, however, show that the vibrational entropy $S_{vib}$ can have a significant effect on solid-state phase transitions. For instance, it is reported that the changes in vibrational entropy about 0.1-0.2$k_B$/atom between two phases $\Delta S_{vib}$ is large enough to have a significant effect on critical temperature, or the shapes of phase boundaries in binary alloys.

**Methods and Materials**: The diffraction data of Ce ingot were obtained using diamond anvil cell (x-ray diffraction) and Al cell (neutron diffraction).

**Results**: We studied elastic properties of γ- and α-phase Ce as a function of pressure using high pressure high resolution neutron and synchrotron x-ray powder scattering. Figure 1 presents bulk modulus of the γ- and α-Ce calculated using the pressure dependence of the lattice parameter (see inset). Figure 2 shows thermal parameter of the γ- and α-Ce as a function of pressure. The thermal displacement drops about 44 % at the transition. This drop of the thermal displacement indicates stiffening of lattice at the transition. More importantly, this result indicates a vibrational entropy change, $\Delta S_{vib}$ = (0.76 ±0.2) $k_B$/atom which more than half of total entropy change at the transition.

**Conclusions**: Anomalous elastic properties and large vibrational entropy change at the phase transition suggest that the lattice plays a role in the phase transition.

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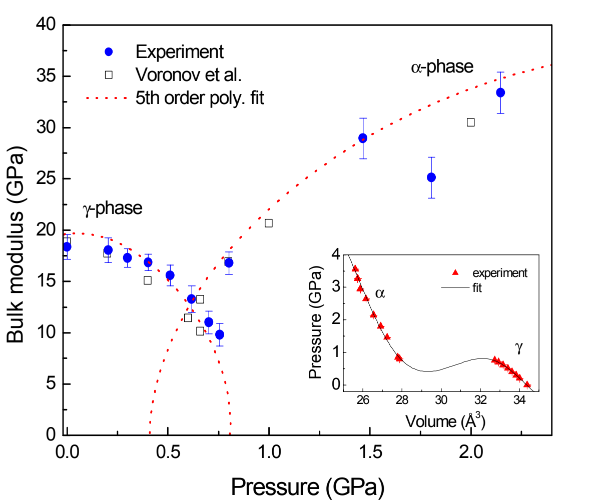


Fig. 1. Bulk modulus of Ce as a function of pressure. Inset shows volume versus pressure.

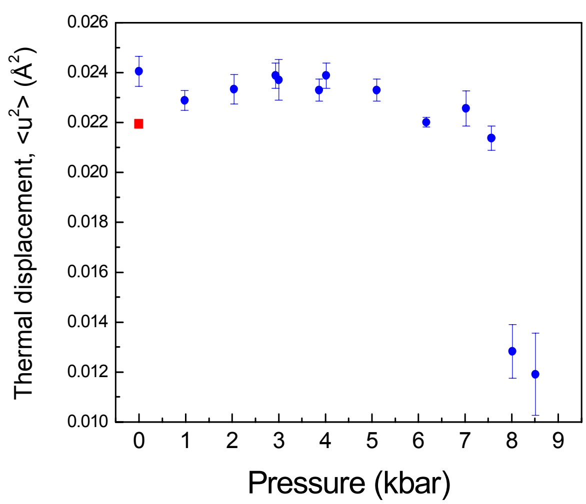


Fig. 2. Thermal displacement of Ce as a function of pressure.