

Lattice dynamics of Cerium metal around the $\gamma \leftrightarrow \alpha$ transition by inelastic X-ray scattering

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Cerium displays an extremely rich and varying behavior under different thermodynamic conditions of temperature and pressure with at least five allotropic forms. The most spectacular transition occurs at a pressure of 8 kbar and 300K between the gamma (low pressure) and alpha (high pressure) phases with a strong volume change of 15% [1]. The current theories suggest that this structural instability is directly linked with the electronic properties of cerium, with the 4f electron being at the border between localisation and itinerancy. Previous measurements of the phonon dispersion of gamma-Ce had shown an unusual softening of the transverse acoustic branch along the [111] and [110] (<110> polarization) directions, which involve the elastic constants C11 and C12, thus explaining the decrease of the bulk modulus with increasing pressure. We performed the first measurements of the longitudinal branches in the gamma and alpha phases close to the transition on the IXS beamline ID28 of the ESRF. We confirmed the anisotropy of the phonon evolution under pressure, with a complex behaviour of the phonon branch in direction [100] (softening with pressure, followed by a hardening close to the transition) and [110] that shows a different behaviour between zone boundary (softening up to the transition) and the rest of the branch (hardening after the transition). With these observations, we open the door to a better understanding of the underlying electronic mechanisms in cerium.

References

- [1] - D.G. Koskenmaki and K.A. Gschneider, Jr. in Handbook on the Physics and Chemistry of Rare Earths, edited by K.A. Gschneider, Jr. and L. Eyring (North-Holland, Amsterdam, 1979), Vol. I, p. 337
- [2] - B. Johansson, I.A. Abrikosov, M. Alden, A.V. Ruban, and H.L. Skriver; Phys. Rev. Lett. 74, 2335 (1995)