A crystallographer’s approach to the mechanism of magnetic C/Tg phase transitions.

P. Becker*, N. Sonnet*, F. Vigneron**

*Institut Laue-Langevin, 156X, 38042 Grenoble Cedex
**Laboratoire Leon Brillouin, Orme des Merisiers, 91190 GIF sur Yvette

Rare earth and rare earth intermetallics reveal a series of magnetic structures, starting from pure halex whose propagation vector may or may not lock in at finite commensurate values. Within a Hamiltonian model which incorporates a competition between exchange interactions and magneto-crystalline effects (anisotropy, magnetostriiction, applied field), it is possible to explain that any incommensurability between the periods of exchange and magneto-crystalline order leads to a singularity in the energy. A strategy is defined to construct the phase diagram. Application to RBe13 intermetallics is discussed in detail and possible generalisations to other magnetic or structural phase transitions are discussed. The method that is used is strongly connected to the crystallographic behaviour of the system, which enables a very simple understanding of the occurrence of transitions.

Pressure favors delocalization and hybridization of f electrons. Thus, the low-symmetry uranium type structure (orthorhombic, Cmcm) was successively observed under pressure in Ce (N.H. Zachariason, F.H. Ellinger, Acta Cryst. A33, 1977, 155-160), in Am (R.B. Roof et al., Science 207, 1980, 1353-1360), in Pr (G.G. Smith, J.A. Akella, J. Less Met. 93, 1979, 95-97), in Bk (R.G. Haire, J. Less Met. 98, 1980, 353-356). These observations confirm the lanthanide-like character of these heavier actinides (i.e., localized f-electrons). Furthermore Ce shows another parallel to the lanthanides: the fcc phase, with further increasing pressure, is distorted (U. Benedict, J. Peterson, R.G. Haire, J. Phys. F: Metal Phys. in press) in a similar way as the fcc phase of Pr, La and Y (W.A. Grosshans, Y.K. Vohra, W.S. Holzapfel, Phys. Rev. Letters 49, 1982, 1572-1570). In particular, Ce and Pr have the same structural sequence dhcp-fcc-distorted fcc-uranium type with increasing pressure. The transition pressure for the dhcp-fcc transition in the actinide series increases with increasing atomic number (Am: 5 GPa, Bk: 7 GPa, Cf: 17 GPa; this is also the case with the earlier lanthanide metals.

05. PHYSICAL PROPERTIES AND STRUCTURE


The sf electrons of the metals Pa, U, Np and Pu are “delocalized” or “itinerant”. This means that they are of band type, hybridize with the other conduction electrons and thus contribute to the metallic bonding. In contrast, the metals Am, Cm, Bk and Cf, which follow in the actinide series, are characterized by sharp sf levels and are said to have “localized” sf electrons which do not participate in the metallic bond.

The delocalization of sf (and 4f) electrons correlates to two phenomena of crystallographic interest:

1) The interatomic distances decrease with respect to the “localized” configuration. Thus, the atomic volumes of the elements Pa to Pu are considerably lower than those of the other actinides. This is due to the extra contribution to the metallic bonding from the sf-band electrons, while in the localized configuration this bonding is absent (B. Johansson, H.L. Skriver, J. Magn. Magn. Mat. 29, 1982, 217-229).

2) Crystal structures of low symmetry appear. U, Np and Pu have a number of orthorhombic and monoclinic structures while the other actinides (with the exception of the body-centred tetragonal Pa) have close-packed cubic and hexagonal structures, at normal pressure and temperature. The appearance of low-symmetry structures is rationalized by a marked directionality of the hybridized orbital, though a quantitative explanation has not yet been given.

With the equipment the kinetics of the phase transitions of YbBr3 have been studied and some interesting results including metastable phases will be presented.