Structure of Cerium above 50 kbar

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In situ x-ray diffraction experiments suggest that above 50 kbar Ce is similar to Ti and Zr which are hexagonal close packed.

A RECENT paper reports a second electronic transition in cerium metal near 50 kbar in which the structure remains fcc but contracts 4% in volume.[1] This phase had previously been reported to become superconducting below 1.7°K.[2] The reported crystallographic transition is not in agreement with our *in situ* x-ray diffraction measurements which show that the phase stable above 50 kbar is very close to the hcp structure. The experimental methods have been described elsewhere,[3] and one of the samples was kindly provided by Wittig. A reversible transition is observed near 50 kbar and the data obtained at a pressure of $\approx$65 kbar are *hkl*, *I*, *d*Å: 100 M 2.728; 002 S 2.603; 101 M 2.411; 102 VW 1.886; 110 M 1.590; 201 W 1.320; 004 VW 1.299; 202 T 1.205; 104(?) *T* 1.116; 203 T 1.070; 211 T 1.023, where S stands for strong, M for medium, W for weak, VW for very weak, and T for trace. The lines can be indexed on a hexagonal cell with $a=3.16\pm0.01$ Å and $c=5.20\pm0.02$ Å. The absence of the 103 reflection and the trace line 1.116 Å suggests that the true structure may be slightly distorted from the simple hcp structure. In fact, only the 110 and 211 reflections give any information about the third dimension of the unit cell. It is reasonable to expect that when the $4f$ levels are no longer populated, Ce should be like Ti and Zr which are hcp at 1 atm and are superconducting. By extrapolation one expects an atomic volume for +4 Ce metal at 65 kbar of 14.1 ± 0.8 cm^3/g atom in reasonable agreement with the observed value of 13.6 ± 0.2 cm^3/g atom. Throughout the rare-earth elements pressure has the same effect as decreasing the number of $4f$ electrons,[4] and in Ce the data suggest it is possible to convert a rare-earth metal into a transition metal by the application of pressure.

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[2] J. Wittig, Phys. Rev. Letters **21**, 1250 (1968).
[3] D. B. McWhan and W. L. Bond, Rev. Sci. Instr. **35**, 626 (1964).
[4] D. B. McWhan and A. L. Stevens, Phys. Rev. **154**, 438 (1967).