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UCRL-CONF-210563

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March 15, 2005

7 International Conference Actinide 2005
Manchester, United Kingdom
July 4, 2005 through July 8, 2005

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1 INTRODUCTION

Actinide physics has seen a remarkable focus the last decade or so due to the combination of improved experimental diamond-anvil-cell techniques and the development of fast computers and more advanced theory. All *f*-electron systems are expected to have multiphase phase diagrams due to the sensitivity of the *f*-electron band to external influences such as pressure and temperature. For instance, compression of an *f*-electron metal generally causes the occupation of *f*-states to change due to the shift of these bands relative to others. This can in some cases, as in the Ce-Th system, cause the crystal to adopt a lower symmetry structure at elevated pressures. Here we study the phase stabilities of Ce, Th, and the Ce-Th system as a function of compression. Theoretically, both Ce and Th metals are rather well described within the DFT,[1] although a proper treatment of the Ce-Th alloys has not yet been presented.[2] In the present paper we revisit this problem by applying the modern theory of random alloys based on the coherent potential approximation (CPA).

2 COMPUTATIONAL DETAILS

The calculations we have referred to as exact muffin-tin orbitals (EMTO) are performed using a full-relativistic Green's function technique based on an improved screened KKR method, where the one-electron potential is represented by optimized overlapping muffin-tin (OOMP) potential spheres[3]. Within the EMTO formalism, the one-electron states are calculated *exactly* for the OOMT potentials. For the exchange/correlation approximation, we use the generalized gradient approximation. For the total energy of random substitutional alloys, the EMTO method has recently been combined with the CPA.[3]

3 RESULTS

In Figures 1 and 2 we plot the calculated *c/a* ratio for bct Ce and Th, respectively. Present results agree well with experimental data[4,5] as well as with those of previous FPLMTO

calculations[1]. Figure 3 shows the calculated (EMTO) and measured[6,7] *c/a* ratios for the $Ce_{43}Th_{57}$ alloy. The results of previous FPLMTO calculations[2] are also presented.

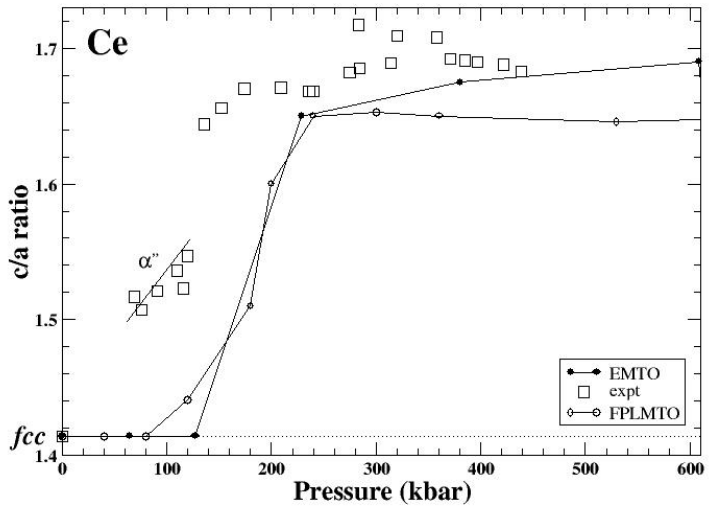

Figure 1 *The c/a axial ratio for the bct structure as a function of pressure for Ce. Experimental data (Ref. 4) are marked with open squares while theoretical results are given by a solid line and filled circles. The results of FPLMTO calculations (Ref. 1) are shown by a solid line and open circles.*

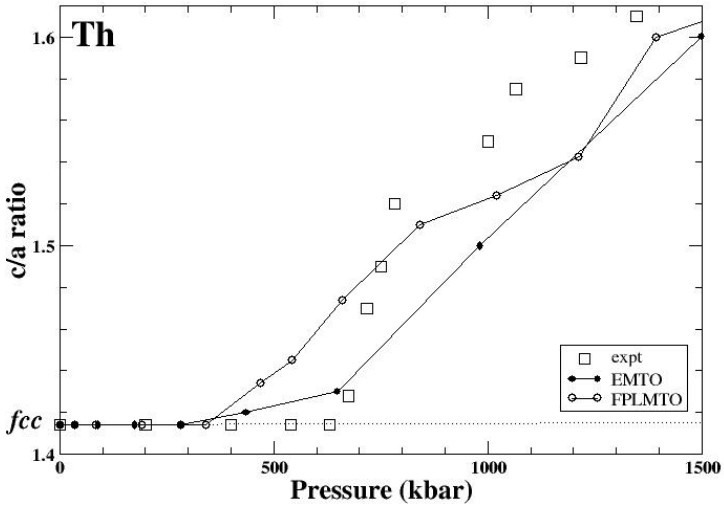

Figure 2 *The c/a axial ratio for the bct structure as a function of pressure for Th. Experimental data (Ref. 5) are marked with open squares while theoretical results are given by a solid line and filled circles. The results of FPLMTO calculations (Ref. 1) are shown by a solid line and open circles.*

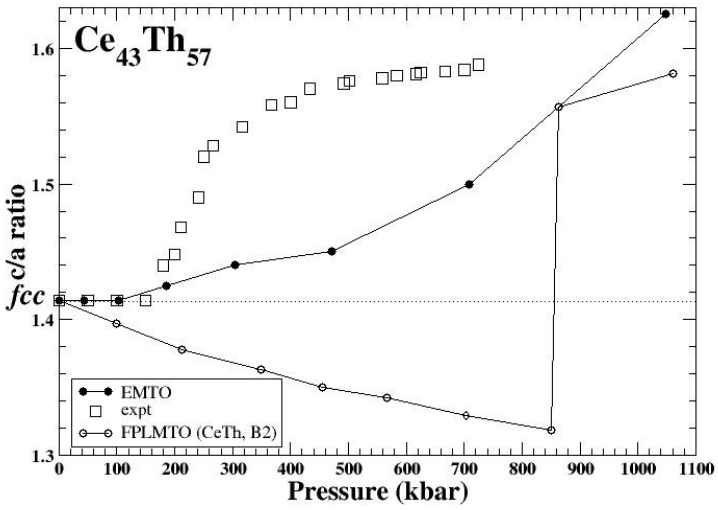

Figure 3 *The c/a axial ratio for the bct structure as a function of pressure for $Ce_{43}Th_{57}$ disordered alloy. Experimental data (Ref. 6, 7) are marked with open squares while EMTO theoretical results are given by a solid line and filled circles. Also, the results of FPLMTO calculations (Ref. 2) for Ce-Th-ordered (B2) compound are given by a solid line and open circles.*

3 CONCLUSION

We have presented accurate electronic-structure calculations for the Ce-Th system. Generally, the theory reproduced experimental data very well. For the $Ce_{43}Th_{57}$ disordered alloy a CPA treatment is necessary to reproduce the correct structural behaviour.

Acknowledgements

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng. 48.

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