Microstrain in δ′-Plutonium

Andrew C. Lawson

In addition to giving information on crystal structure, the shapes of the diffraction peaks also give valuable information on other aspects of the state of the material. In particular, if the lattice "constant" is not really constant but actually fluctuates throughout the bulk material, then the diffraction lines will be broadened. One mechanism for fluctuation is the strain caused by the forces exerted by the grains on one another in the course of a crystallographic transformation.

Thanks to the analysis developed recently by Peter Stephens, it is now possible to include anisotropic microstrain broadening in the Rietveld analysis. This means that one allows for the strain in individual grains to depend on crystal direction. The observed microstrain, which is an average over many grains, is a distribution that must be consistent with the crystal symmetry. The observed microstrain in δ′-plutonium is shown in Figure 1. The figure indicates that the spread in the distribution of lattice spacings is much greater in the crystallographic *c*-direction of the tetragonal crystals of δ′-plutonium than in the *a*-direction.

Why is the microstrain so high for δ′-plutonium? We do not know in detail, but it would seem that the tetragonal δ'-structure is a rather unhappy compromise between the two cubic structures, δ and ε (Figure 2).

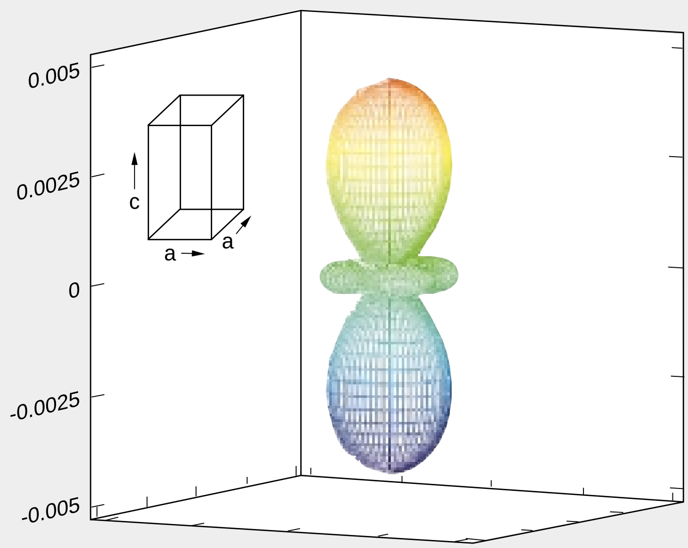

Figure 1. Anisotropic Microstrain for δ′-Plutonium at 740 K
This plot shows the root-mean-square average deviation of the crystal *d*-spacings in δ′-Pu plotted versus crystal direction. This quantity is called the microstrain, and it is determined by intergranular stresses. In the tetragonal crystal shown here, the microstrain is much larger in the crystallographic *c*-direction. The microstrains are caused by intergranular stresses.

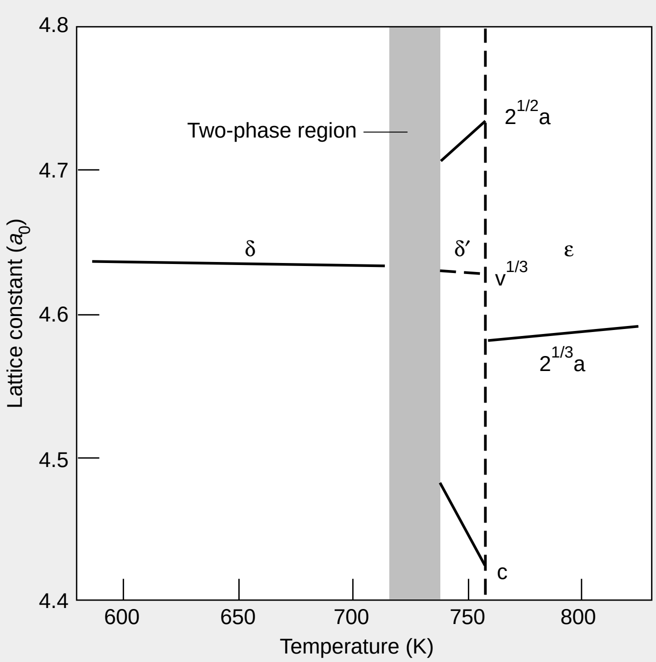

Figure 2. Temperature Dependence of the Normalized Lattice Constants of Pure Plutonium
Between 600 and 800 K, plutonium transforms from face-centered-cubic δ′-phase to face-centered-tetragonal δ′-phase and then to body-centered-cubic ε-phase. Even though they are both cubic, the structures of the δ′- and ε-phases are not closely related to each other, and the atomic volumes are very different. The interatomic distances have to change considerably during the transformation, and this change leads to a large microstrain for the tetragonal δ′-phase. **(Reproduced with permission from *Kluwer Academic*, A. C. Lawson et al., Edited by A. Gonis et al., "Light Actinides" in *Electron Correlation and Materials Properties*, 1999, page 75.)**