

**s11.m33.p1** **The fcc-bcc Bain Path in Binary Alloys Under High Pressure: Valence Electrons as a Driving Force.** Valentina Degtyareva, *Institute of Solid State Physics Russian Academy of Science, Chernogolovka, Russia. E-mail: degtyar@issp.ac.ru.*

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The structural transformation from face-centered cubic (*fcc*) to body-centered cubic (*bcc*) is known as the Bain path. Both structures can be represented by a common tetragonal cell: *bct* (*fc**t*) with  $c/a = \sqrt{2}$  and 1 (1 and  $1/\sqrt{2}$ ) for *bcc* and *fcc*, respectively. Transitions between *fcc* and *bcc* occur in iron-carbon alloys by temperature quenching and in some metals upon heating and/or compression. Related to the Bain path tetragonal phases are shown to form in the epitaxial metal films in order to release the stress due to the size mismatch. The driving forces behind these transitions originate from an external force such as temperature, pressure or strain.

In our work we consider a sequence of tetragonal phases in binary *sp* metal alloys that provides strong evidence for a correlation of *c/a* with an alloy composition or electron to atom ratio - an internal parameter. A driving force behind the tetragonal distortion in these alloy phases is associated with the number of valence electrons per atom. Tetragonal structures of metallic phases are considered in In-Sn and related alloys including data on equilibrium ambient-pressure phases; metastable phases quenched from liquid and high-pressure phases obtained in our studies [1-6]. Degree of tetragonal distortion from *fcc* or *bcc* is related to the valence electron concentration (*z*) within a model of the Brillouin zone - Fermi surface interaction (FSBZ). To analyse the features of the *fcc* - *bcc* transformation path in *sp* metal alloys two contributions to crystal energy need to be considered: the electrostatic Ewald term and the electron contribution due to FSBZ. It was suggested that for In and In alloys it is favourable for BZ corners to touch the Fermi sphere. This results in the instability of *fcc* with respect to tetragonal distortion. According to this model the axial ratio adapts itself to maintain this contact following the expanded FS caused by alloying. Application of high pressure shifts the balance between the two terms of the crystal energy making the electronic contribution increasingly dominant. Our results on binary alloys under pressure correspond well this FSBZ model: (i) *fcc* - *fc**t* transitions under pressure in the In-Pb alloys with 40 and 60 at.% Pb [4]; (ii) pressure-induced decomposition of the  $\text{In}_5\text{Bi}_3$  compound into two tetragonal phases with different *c/a* [5]; (iii) a switch from  $c/a > 1$  to  $c/a < 1$  in the In-10 at.% Pb alloy on compression [6].

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**s11.m33.p2** **Monoclinic Phases of Ce and Pr: Crystal Structure and Thermodynamical Stability.** Vladimir Dmitriev<sup>a</sup>, Alexey Kuznetsov<sup>b</sup>, Olga Bandilet<sup>c</sup>, Pierre Bouvier<sup>c</sup>, Leonid Dubrovinsky<sup>b</sup>, Denis Machon<sup>d</sup> and Hans-Peter Webera<sup>e</sup>, <sup>a</sup>Group "Structure of Material under Extreme Conditions", Swiss-Norwegian Beam Lines at ESRF, France, <sup>b</sup>Bayerisches Geoinstitut, Universität Bayreuth, Germany, <sup>c</sup>LPMI, INPG-CNRS, France, <sup>d</sup>Department of Chemistry, University College London, UK, <sup>e</sup>Laboratoire de Cristallographie, Swiss Federal Institute of Technology, Switzerland. E-mail: dmitriev@esrf.fr

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Pressure-induced structural phase transformations in rare-earth metals Ce and Pr were studied at different temperatures by angle dispersive x-ray diffraction using a synchrotron source. Our study definitely evidenced the existence of the monoclinic phase, Pr-VII, in the pressure range 10 to 25 GPa, intermediate between the distorted *fcc*, Pr-III, and the orthorhombic, Pr-IV, phases. The monoclinic structure belonging to the C2/m space group (*Z*=8) and the unit cell lattice parameters:  $a=10.984(2)$  Å,  $b=6.3810(2)$  Å,  $c=6.275(3)$  Å and  $\beta=126.12(1)$ . The Pr atoms occupy two 4-fold positions and one general 8-fold position with the atomic positional parameters: 4(i)<sub>1</sub>: (0.7149, 0, 0.2666), 4(i)<sub>2</sub>: (0.2338, 0, 0.2680) and 8(j): (-0.0107, 0.7589, 0.2655). The above monoclinic structure, Pr-VII, gives good reliability indices ( $R_{wp}=0.0383$ ,  $GoF=1.62$ ) even without a preferred orientation correction. The symmetry analysis shows that the same, as for the *fcc*-dist.*fcc* and *fcc*- $\alpha'$ -Ce transformations, the longitudinal phonon instability induces the transition into the monoclinic Pr-VII phase. The phenomenological models worked out for the above transformations reproduce well the topology of the phase P-T diagrams of Ce and Pr, and relates the high lability of the  $\alpha'$ -Ce- $\alpha$ -U phase boundary to the identity of their distortion mechanisms. It was shown earlier, in the framework of the unified crystallographic scheme [1], that all displacive transformation mechanisms, which give rise to the lanthanide structures, are the variants of the Burgers and Bain deformations of the *bcc* parent phase. The  $\alpha$ -U and  $\alpha'$ -Ce structures provide the link between two above mechanisms. We show that  $\alpha$ -U and  $\alpha'$ -Ce structures are the originally equivalent domains of the same orthorhombic phase distorted, due to its different orientation, in different manner by the "external field" of the Bain deformation.

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