



	<b>Experiment title:</b> <b>Polytypism of Pr metal: stable disordered polytype structure</b>	<b>Experiment number:</b> <b>HS 1362</b>
<b>Beamline:</b> BM1A	<b>Date of experiment:</b> from: 22/02/2001 to: 25/02/2001	<b>Date of report:</b> 05/10/2001  <i>Received at ESRF:</i>
<b>Shifts:</b> 6	<b>Local contact(s):</b> Dr. Jon Are BEUKES	
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## Report:

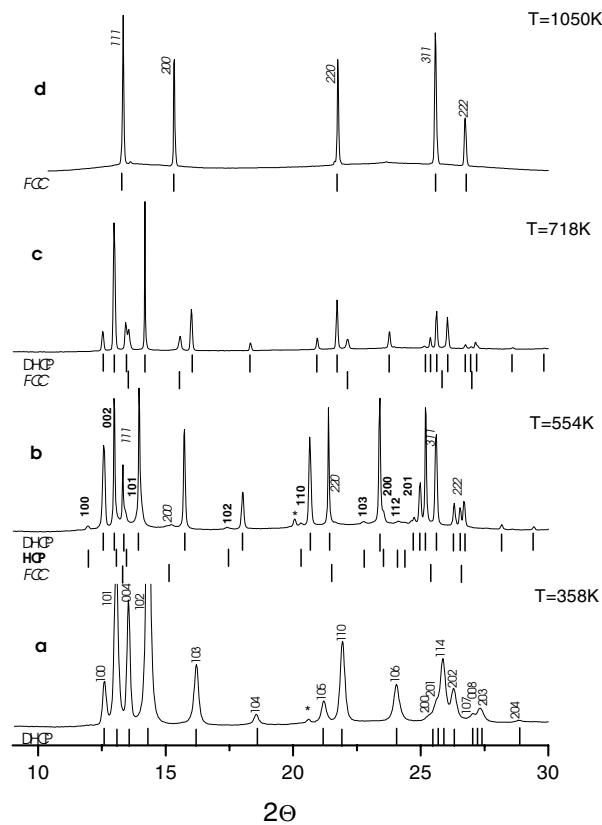
The existence of a body centered cubic (bcc) structure in the high-temperature region of the phase diagram of almost all lanthanide metals suggest a displacive type mechanisms of transformations with the bcc structure as a parent one. On the other hand, the existence of double and triple hexagonal close-packed (hcp) polytypes, or of 9R structures, in most of the lanthanide phase diagrams denotes a strong tendency to polytypism, which is associated with a reordering process, involving a disordered polytype structure [1, 2]. Detection of a disordered polytype phase in the phase diagram of a lanthanide metal would be a decisive experimental discovery allowing to chose a primary (symmetry - breaking) mechanism for the low pressure transformations in rare-earth metals.

In the latter case phenomenological considerations predict the existence of such a disordered phase in Pr [2]. Moreover, the experimental data published on the dhcp-fcc phase stability boundaries in Pr [3] allowed us to map the corresponding stability domain, which had been predicted theoretically, on the experimental pressure-temperature phase diagram of Pr metal [2]. This stability region of the disordered polytype has been so far investigated by different experimental techniques (see review paper [4] and

references therein), but studies failed to produce conclusive results, which led the authors of Ref. 4 to designate this part of phase diagram as an uncertainty area.

We carried out the high-temperature (at ambient pressure) and high-pressure (at ambient temperature) studies of Pr metal concentrating our attention on the region of uncertainty in the phase diagram. We employed two types of set-up for temperature measurements: first, one with a Lincam DT-1500 cell, and, second, one with the ETH-800 furnace. Both arrangements provide the control of an atmosphere in the sample holder (it was an argon of high purity in our case). A diamond anvil cell was used in pressure experiments. All samples were prepared and loaded in glove box to avoid an oxidation of Pr at room temperature.

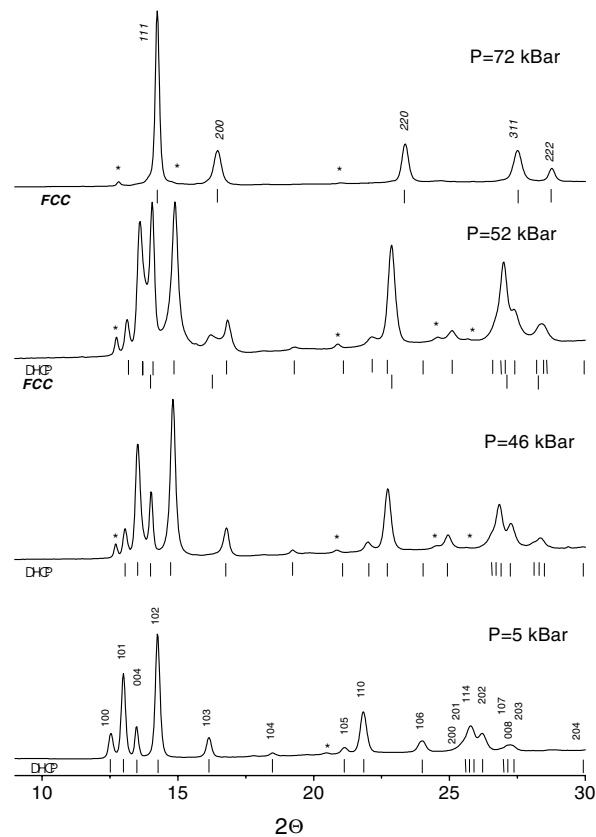
The angle dispersive X-ray diffraction technique was used to obtain the intensity versus  $2\theta$  data. Fig. 1 and 2 show the evolution of the spectrum of Pr with temperature and pressure. One can conclude that relying on the results obtained the region of uncertainty in phase diagram of Pr is the region of coexistence of dhcp and fcc phases. Unfortunately, lack of time did not permit us to check the possible delay in the formation of the presumed disordered polytype structure due to kinetics of this process. In all tests we clearly observed the formation of new peaks, indexed as belonging to an hcp lattice (see Fig. 1), in the temperature range of



**Fig. 1.** Evolution of diffraction spectrum of Pr with temperature (pressure is ambient). Asterisks indicate the positions of peaks of praseodymium oxide.

interest. The lattice parameters of hcp phase have a strong correlation to the lattice parameters of dhcp phase of Pr ( $a_{\text{hcp}} \approx a_{\text{dhcp}}$  and  $c_{\text{hcp}} \approx 0.5 \cdot c_{\text{dhcp}}$ ). This fact suggests a close connection between these phases and we need

to study this relationship in greater detail, together with an additional investigation of kinetics of phase transition from dhcp to fcc in Pr. It should be noted that the temperature range of coexistence of dhcp and fcc phases at ambient pressure (from about 550 to 900 K in this experiments) does not show a narrowing of hysteretic region separating the fcc and dhcp phases, in contrast to data of Ref. [3].



**Fig. 2.** Evolution of diffraction spectra of Pr with pressure (temperature is ambient). Asterisks indicate the positions of peaks of praseodymium oxide.

## References

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