The two phase diagrams for PdD

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The phase diagram of PdH (and also PdD) has been studied extensively over the past century or more, and is considered to be well understood. However, there is a subtle issue in connection with the phase diagram this is not well understood; this has to do with the stability of the lattice itself, in connection with the different phases.

In the literature, one usually finds the phase diagram for conditions under which the Pd sub-lattice is assumed to be fixed. Given the long relaxation time associated with vacancy diffusion under "normal" conditions, the phase diagram that results is very useful.

However, the addition of H or D causes the vacancies to be stabilized, so at sufficiently high loading the thermodynamic equilibrium favors the vacancy phase. At low or modest temperature this entails no consequence, since in general it is very hard for the vacancy phase to form. However, at higher temperature one would expect the vacancy phase to form, so the vacancy phase will be an important part of the diagram. At lower temperature, the vacancy phase can form through codeposition if the loading is sufficiently high.

It seems useful given this situation to discuss the phase diagram at low temperature under conditions where codeposition can form new lattice, in order to emphasize that the new material can be very different than what lies underneath as a consequence of the phase diagram. In a sense, we really need two phase diagrams to understand PdD.