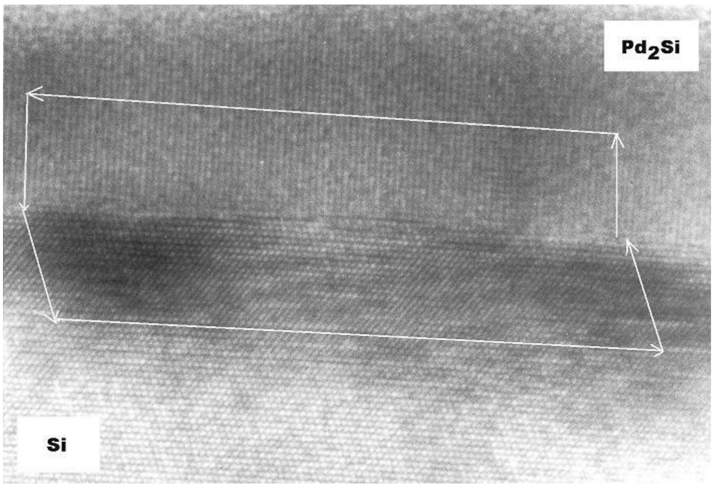
8.2.2 Case Study for Pd Silicides

- If **Pd** instead of **Ni** is evaporated on a clean **Si** surface, hexagonal **Pd_2Si** (***a* = 0,653 nm**, ***c* = 0,344 nm**) develops around **200°C - 300°C**. Increasing the annealing temperatures produces no new phases.
  - The misfit of the hexagonal **{001}** plane to a **Si {111}** plane is **1,8%**; we can expect an epitaxial relationship with a misfit dislocation network at a spacing of about **10 nm**. This is around the resolution limit of **TEM** in a regular contrast mode, so we have to resort to **HRTEM** and cross-sectional specimen.
  - A **HRTEM** image of the interface is shown below (*This picture from **1980** is of historical interest, too: It was, to the best of my knowledge, the first **HRTEM** picture ever obtained from a phase boundary*).



- We clearly have an epitaxial layer of **Pd_2Si**. No ending lattice fringes denoting misfit dislocations are unambigously visible. Therefore a Burgers circuit has been drawn, somewhat analogous to the procedure used to obtain Franks formula. It goes up in the **Pd_2Si**, then to the left crossing **90** lattice fringes, back to the boundary, **90** fringes to the right and up to the boundary again. It does *not* close, although it is clear that it would have closed on a perfectly flat and misfit-dislocation free interface.
  - Does this mean that the phase boundary contains misfit dislocations?
  - This is not clear. We *may* have dislocations in the interface, but we *certainly* have steps as can be seen directly. We now have to pay some attention to the *relationship of dislocations and steps*, their images in a **HRTEM** picture, and their consequences for a Burgers circuit.
- This will lead us into new and quite complicated territory. We will consider the relationship between steps and dislocations only for the example of hexagonal lattices on cubic lattices, or, more generally, for **$\Sigma = 3$** relations. This will be sufficient to gain an idea of the added complexity.