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Local atomic arrangements in Ni-Pt

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The microstructure of the bulk and surface of Ni-Pt alloys has attracted much interest over the years. For Ni-Pt surfaces, the segregation reversal is the most striking feature, with Ni enrichment for the top layer of a (110) surface and Pt enrichment for the top layer of (110) and (111) surfaces. Strong ordering for nearest neighbors and the different strength of Pt segregation into different layers were found as being the reason. For bulk Ni-Pt, ab initio electron structure calculation and x-ray diffuse scattering both revealed the presence of a new phase, NiPt3 with L12 superstructure, below about 400°C.

To investigate the region between surface and bulk, diffuse x-ray scattering under grazing incidence was done. Here, the (100) and (110) surfaces of Ni-23 at.% Pt were measured for states above the bulk order-disorder transition temperature. The atomic arrangements always show local L12 features. As the microstructure is no longer homogeneous close to the surface due to surface segregation and relaxation, additional information from literature / from crystal truncation rods (fundamental and superstructure) is required to model the atomic arrangements.

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