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Successive transitions to modulated states in the {R}Pt₂Si₂ family

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Materials with low electronic dimensionality are known to exhibit remarkable properties such as thermoelectricity, high electron mobility or superconductivity. In addition, this low dimensionality also favors the appearance of another phenomenon: charge density wave instability (CDW). The transition to a CDW state is described by Peierls [1] as a gap opening at the Fermi Surface of the material leading to the modulation of its electronic density accompanied by a periodic distortion of its atomic lattice. Therefore, a transition to a CDW state is characterized by the appearance of an anomaly in the electron transport properties and of additional reflections in the X-ray diffraction pattern, called satellite reflections.

A resistive signature, characteristic of a CDW transition, was observed for the compounds {R}Pt₂Si₂, with R = La, Nd and Pr, at 112 K, 77 K and 88 K respectively [2,3]. The thermal study of the X-ray diffraction pattern of these materials reveals not only the appearance of satellite reflections associated with the reported CDW transitions but also the existence of another transition, at higher temperature, leading to a modulated structure [4,5]. This unexpected phase transition, for which no anomaly in the electron transport properties is observed, is characterized by the appearance of an incommensurate modulation characterised by the wave vectors $\mathbf{q}_1 = 0.360\mathbf{a}^*$, $0.323\mathbf{a}^*$ and $0.326\mathbf{a}^*$ for LaPt₂Si₂, NdPt₂Si₂ and PrPt₂Si₂, respectively. In the case of LaPt₂Si₂, this vector is very similar to the nesting vector of a CDW transition determined by *ab initio* calculations [6]. At lower temperature, a new set of satellites appears, coexisting with the first one, corresponding to the CDW transition reported in the literature and characterized by the wave vectors $\mathbf{q}_2 = (0.187; 0.187; 0.5)$; $(0.158; 0.158; 0.5)$ and $(0.168; 0.168; 0.5)$ for LaPt₂Si₂, NdPt₂Si₂ and PrPt₂Si₂, respectively.

These observations raise a new question: what is the nature of the first structural transition of {R}Pt₂Si₂?

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