MS21-1-1 {R}Pt_2Si_2 family: a modulated story
#MS21-1-1

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Abstract
Materials with low electronic dimensionality are currently widely studied due to their natural tendency to exhibit remarkable properties such as thermoelectricity, high electron mobility or superconductivity. Moreover, this low dimensionality is also at the origin of another phenomenon: the charge density wave instability (CDW). This instability can be described by Peierls' theory [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.
An anomaly in the resistivity measurements, signature of a CDW transition, was reported at 112 K, 77 K and 88 K for the compounds {R}Pt_2Si_2, with R = La, Nd and Pr respectively [2,3]. However, no structural transition was evidenced by powder X-ray diffraction [4] and only one approximate modulation vector has been determined for $LaPt_2Si_2$ by electron diffraction: $\mathbf{q}$ = 1/3 $\mathbf{a^*}$ [3]. To understand the structural impact of these CDWs we performed a single-crystal X-ray diffraction study on these materials at low temperature. This study reveals not only the appearance of satellite reflections associated with the reported CDW transitions but also the existence of an additional transition, at higher temperature, leading from an unmodulated structure to a modulated structure [4 ,5]. This unexpected phase transition, corresponding to no reported resistive anomaly, leads to an incommensurate structural modulation characterised by the wave vectors $\mathbf{q_1}$ = 0.360 $\mathbf{a^*}$, 0.323 $\mathbf{a^*}$ and 0.326 $\mathbf{a^*}$ for $LaPt_2Si_2$ ($160\ K < T_1 < 150\ K$), $NdPt_2Si_2$ ($300\ K < T_1 < 260\ K$) and $PrPt_2Si_2$ ($290\ K < T_1 < 120\ K$) respectively. In the case of $LaPt_2Si_2$, this vector is very similar to the nesting vector of a CDW transition determined by ab initio calculations [6]. This observation stands in favour of a CDW-nature of the first structural transition. At lower temperature, a new set of satellites appears, coexisting with the first one, corresponding to the CDW transition observed in the resistivity measurements. This additional modulation is characterized by the wave vectors $\mathbf{q_2}$ = α $\mathbf{a^*}$ + α $\mathbf{b^*}$ + 0.5 $\mathbf{c^*}$; with α = 0.187; 0.158 and 0.168 for $LaPt_2Si_2$ ($115\ K > T_2 > 100\ K$), $NdPt_2Si_2$ ($90\ K > T_2 > 40\ K$) and $PrPt_2Si_2$ ($110\ K > T_2 > 90\ K$) respectively. Last but not least, a third set of satellite reflections, with the wave vector $\mathbf{q_3}$ = 0.094 $\mathbf{a^*}$ + 0.094 $\mathbf{b^*}$ + 0.25 $\mathbf{c^*}$, is observed on the XRD pattern of $LaPt_2Si_2$ at 50 K, showing that this familly is still full surprises and deserves more investigations.

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