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Coupled structural collapse and evolution of magnetic phases in $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ under pressure

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Abstract

We report high-pressure x-ray diffraction and electrical resistance measurements on $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$, an itinerant antiferromagnet with the highest Néel temperature ($T_N = 36$ K) among $\text{Sr}(\text{Co}_{1-x}\text{Ni}_x)_2\text{P}_2$ series. Room-temperature diffraction data reveal a pressure-induced transition from an uncollapsed tetragonal to a collapsed tetragonal (cT) structure, beginning near 8.4 GPa and completing before 12.4 GPa. This transition is characterized by an expansion of the in-plane a -lattice parameter and a contraction in the c -lattice parameter, resulting in a reduction of the axial ratio c/a . Resistance measurements show a low-pressure anomaly near 38 K, consistent with the reported antiferromagnetic transition. As the room temperature value of the applied pressure exceeds 8 GPa, signs of a partial cT transition appear on cooling with the full cT transition occurring for pressures exceeding 10 GPa. The cT phase is accompanied by a much higher-temperature transport anomaly that resembles the pressure-induced ferromagnetic transition reported for SrCo_2P_2 , reaching approximately 190 K before gradually decreasing at higher pressures. These results demonstrate strong coupling between the lattice collapse and magnetic behavior in $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$.

1. Introduction

Compounds of the form AT_2Pn_2 , where A is an alkali, alkaline-earth, or rare-earth metal, T is a transition metal, and Pn is a pnictogen, frequently crystallize in the ThCr_2Si_2 structure [1]. This layered structure has been studied extensively, providing important insights into materials with highly tunable structural, magnetic, electronic, and superconducting properties [2]. In particular, the bond strength between adjacent Pn atoms has been a major focus because of its strong influence on the crystal structure of these materials [1, 2]. Many of these systems exhibit a pressure-induced isostructural phase transition characterized by a large compression along the c -axis accompanied by a smaller expansion of the in-plane lattice parameter a . The resulting phase is known as the collapsed tetragonal (cT) phase, and is generally associated with a drastic collapse of the c -axis and formation of interlayer $\text{Pn} - \text{Pn}$ bonding, which is absent in the uncollapsed tetragonal (ucT) phase [1, 3–7]. Previous studies have provided strong evidence for significant coupling between the structural changes associated with this phase transition and the electronic and magnetic properties of these materials [8–15].

The ucT–cT phase transition can be tuned experimentally through chemical doping [14, 16–19], external pressure [2, 20–22], and uniaxial strain [23, 24]. Owing to the high tunability of the interlayer Pn distance, these systems can host superconducting, antiferromagnetic (AFM), ferromagnetic (FM), or nonmagnetic ground states [2, 3, 9, 20, 25]. Recent studies of Co-substituted $\text{Sr}(\text{Ni}_{1-x}\text{Co}_x)_2\text{P}_2$ have shown that chemical substitution strongly modifies both the structural and magnetic ground states:

although the parent compound SrNi_2P_2 does not exhibit long-range magnetic order at ambient pressure [16], magnetic order emerges at intermediate Co concentrations before disappearing again near the SrCo_2P_2 end member [16, 20, 26–28]. In addition, external pressure monotonically suppresses bulk superconductivity in SrNi_2P_2 [20]. An applied pressure of ~ 10 GPa drives pure SrCo_2P_2 into the cT phase with an accompanying FM transition near room temperature [12]. Together, these results highlight the strong coupling between bonding, structure, and emergent electronic and magnetic properties in these layered pnictides.

The previous studies raise the question of whether pressure can similarly tune the structural and magnetic behavior of Co-substituted $\text{Sr}(\text{Co}_{1-x}\text{Ni}_x)_2\text{P}_2$ near the boundary between AFM and FM order. This question is particularly relevant for $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$, whose composition lies close to the maximum reported AFM transition temperature and near the crossover toward FM behavior with decreasing Ni concentrations [16]. Motivated by this chemical substitution phase diagram and by the demonstration of pressure tunability of SrCo_2P_2 [12], we performed pressure-dependent x-ray diffraction (XRD) and electrical resistance measurements to establish a temperature-pressure phase diagram of $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$.

2. Experimental methods

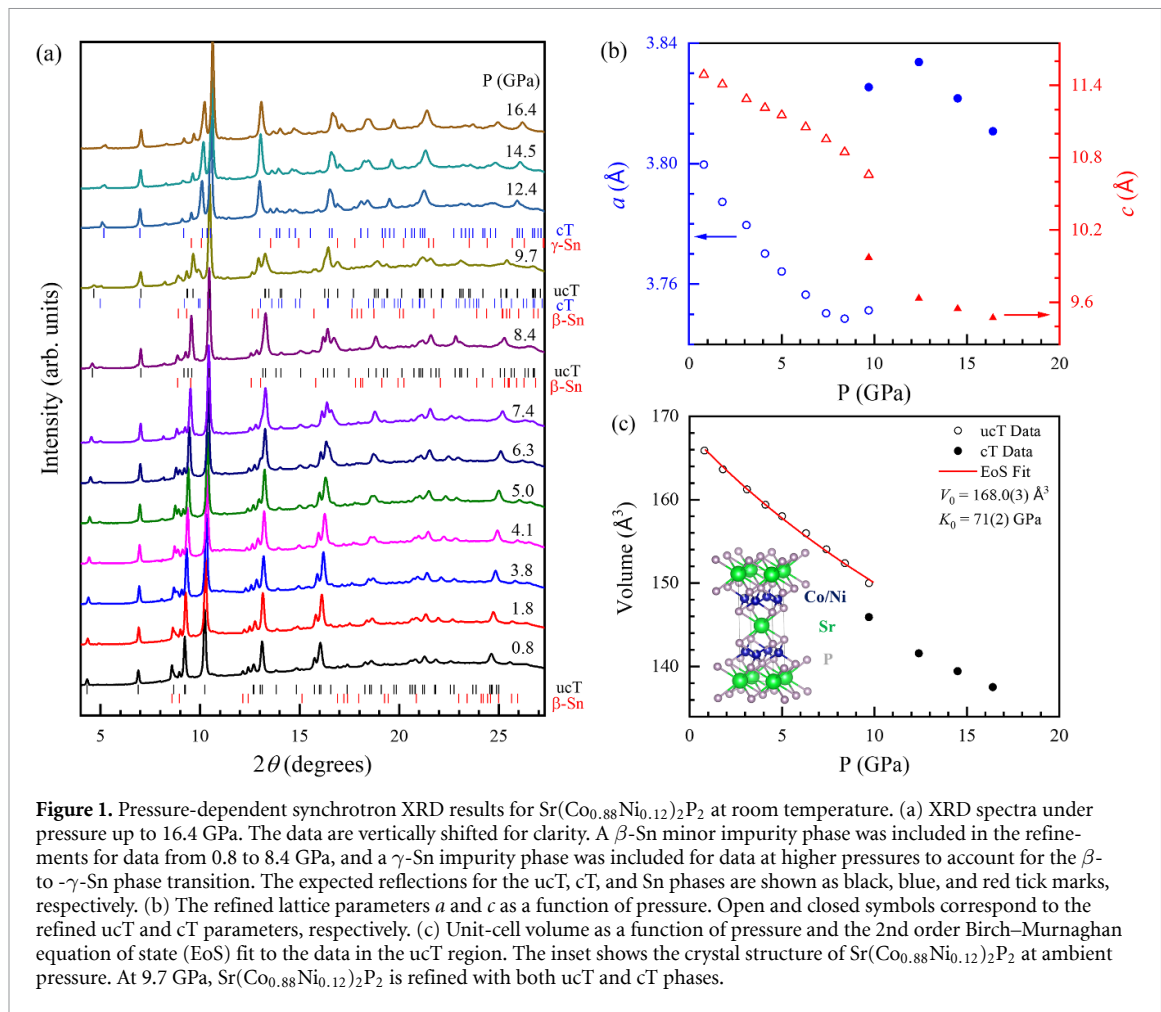
Single crystals of $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ were synthesized using the high-temperature solution growth out of Sn flux [16]. High-pressure angular-dispersive synchrotron XRD experiments were performed at room temperature at Beamline 13BM-C of the Advanced Photon Source, Argonne National Laboratory. The x-ray wavelength was set to $\lambda = 0.434$ Å and the x-ray beam was focused to a $15\text{ }\mu\text{m}$ (v) $\times$ $15\text{ }\mu\text{m}$ (h) size. Pressure was generated using a BX90 diamond anvil cell (DAC) [29] equipped with diamond anvils of $500\text{ }\mu\text{m}$ diameter culet. A rhenium gasket with an initial thickness of $250\text{ }\mu\text{m}$ was preindented to approximately $80\text{ }\mu\text{m}$ thick, and a $250\text{ }\mu\text{m}$ diameter hole was laser-drilled to form the sample chamber. Powder samples were loaded together with neon as the pressure-transmitting medium and pressure was determined from the ruby R1 fluorescence line [30, 31]. The two-dimensional diffraction images were integrated using DIOPTAS software [32]. The powder sample was prepared by crushing single crystals, but the small illuminated volume in the DAC contained a limited number of crystallites. Consequently, the two-dimensional diffraction images exhibited discontinuous and azimuthally nonuniform Debye–Scherrer rings, indicating insufficient powder averaging. The integrated reflection intensities also showed variations that may arise from preferred orientation and changing grain statistics under pressure. Because reliable Rietveld refinement requires accurate relative integrated intensities, refinement of atomic coordinates and occupancies was not considered sufficiently constrained. Le Bail refinement, which fits peak positions and intensities without refining a structural model, was therefore performed using GSAS-II [33] to extract the pressure-dependent lattice parameters.

Electrical resistance measurements were performed in a standard linear four-probe configuration with current applied within the *ab* plane using a Quantum Design physical property measurement system (PPMS). High-pressure measurements were carried out using a Cu–Be DAC compatible with the PPMS. Standard-cut type Ia diamond anvils with $500\text{ }\mu\text{m}$ culet were used. Single crystal samples were cleaved and cut into a rectangular shape with typical dimensions of approximately $110 \times 40 \times 15\text{ }\mu\text{m}^3$, and loaded into an apertured stainless-steel gasket. The gasket was electrically insulated with cubic boron nitride mixed with epoxy. The gasket hole diameter was approximately $160\text{ }\mu\text{m}$. Thin platinum foils were used as electrodes to establish electrical contact with the sample. Nujol mineral oil was used as the pressure-transmitting medium to achieve a quasi hydrostatic pressure environment with a small pressure gradient [34–36]. Resistance data were taken upon cooling with pressure measured at room temperature using ruby fluorescence.

3. Results and discussion

3.1. Pressure-induced structural transition

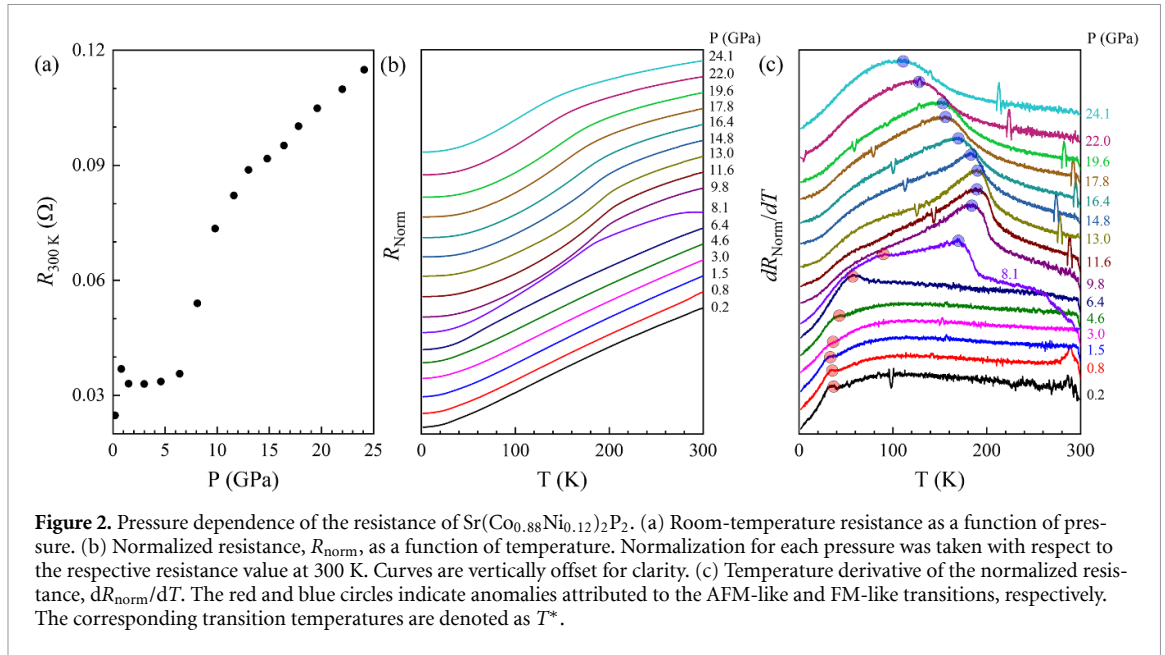
The pressure evolution of the XRD spectra and lattice parameters obtained from Le Bail refinements of synchrotron XRD measurements are summarized in figure 1. At ambient pressure, $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ crystallizes in the uCT (*I4/mmm*) structure [16]. As shown in figure 1(a), the XRD data from 0.8 to 8.4 GPa can be refined with the uCT phase together with a minor β -Sn (*I4₁/amd*) impurity phase from the residual Sn flux. Both lattice parameters and the unit cell volume initially decrease monotonically under pressure, as expected for lattice contraction. Above 8.4 GPa, however, the lattice parameter *a*



deviates slightly from this trend, decreasing somewhat more slowly with increasing pressure, while c decreases more rapidly. Between 8.4 and 12.4 GPa the cT transition takes place with a small expansion of the a -lattice parameter and a significant decrease in the c -lattice parameter. For pressures higher than 12.4 GPa, the lattice experiences normal compression again. At 9.7 GPa, a mixture of ucT and cT phases is required to refine the data. Because Sn undergoes a β - to γ -Sn ($I4/mmm$) phase transition at pressure near 10 GPa [37], the γ -Sn phase was included in the data refinements at 9.7 GPa and above (figure 1(a)). The extracted a - and c -lattice parameters from both the ucT and cT phases are included in figure 1(b). Based on these data, we conclude that the cT phase transition occurs very close to 11 GPa at room temperature.

As shown in figures 1(c) and (a) corresponding discontinuity in the unit cell volume is observed over the same pressure range. To quantify the compressibility of the ucT phase, the pressure dependence of the unit-cell volume up to 9.7 GPa was fitted using the second-order Birch–Murnaghan EoS, as shown in figure 1(c). The fit yields an ambient-pressure unit-cell volume of $V_0 = 168.0(3) \text{ \AA}^3$ and a bulk modulus of $K_0 = 71(2) \text{ GPa}$. Direct experimental EoS values are not readily available for the ucT phases of SrCo_2P_2 or SrNi_2P_2 . For comparison, the related ThCr_2Si_2 -type phosphide LaRu_2P_2 has reported bulk moduli of 105(2) GPa in the ucT phase [5], whereas a low-pressure value of 72(3) GPa has been reported for EuNi_2P_2 [38]. The bulk modulus value is therefore comparable to that of EuNi_2P_2 but lower than that of LaRu_2P_2 in the ucT phase.

In the cT phase, the experimental volume deviates from the EoS fit, consistent with the ucT–cT transition. Above 12.4 GPa, the lattice parameters and unit-cell volume resume a monotonic decrease up to the highest measured pressure of 16.4 GPa. Because Le Bail refinements do not model atomic positions, the P–P distance was not extracted here. The abrupt decrease in c and c/a , together with the volume discontinuity, is nevertheless consistent with the ucT–cT transition and associated interlayer bonding established in related ThCr_2Si_2 -type compounds [39, 40].



3.2. Electrical resistance under pressure

To gain insight into the evolution of the electronic and magnetic state, we performed electrical resistance measurements under pressure up to 24.1 GPa. Figure 2(a) shows the pressure dependence of resistance at room temperature, $R_{300\text{K}}$. At low pressures, $R_{300\text{K}}$ changes weakly. A pronounced increase in resistance then starts near 8.1 GPa, increases even faster at 9.8 GPa, and approaches a more linear increase by 11.6 GPa, coincident with the changes in the a - and c -lattice parameters identified from the XRD measurements. Upon further compression, $R_{300\text{K}}$ continues to increase monotonically up to the highest measured pressure of 24.1 GPa. This increase may reflect changes in carrier density, mobility, scattering, or Fermi-surface reconstruction associated with the structural collapse.

Similar behavior was reported for the parent compound SrCo_2P_2 under pressure [12]. In that study, density functional theory (DFT) calculations showed that the structural collapse is accompanied by substantial changes in the electronic structure, including depopulation of $\text{P } p_z$ antibonding states and an enhanced density of states near the Fermi level associated primarily with $\text{Co } d_{xy}$ character. The latter was proposed to promote an itinerant FM instability in the cT phase. By analogy, the increase in resistance observed here in $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ may reflect a pressure-induced reconstruction of the electronic structure associated with the onset of lattice collapse.

The normalized resistance, defined as $R_{\text{norm}}(T) = R(T)/R_{300\text{K}}$ at each pressure, is plotted as a function of temperature at each pressure in figure 2(b). The normalization facilitates comparison of the temperature dependence across pressures. At low pressures, $R_{\text{norm}}(T)$ exhibits a weak anomaly that is more clearly resolved in the temperature derivative, dR_{norm}/dT , as shown in figure 2(c). This feature appears near 38 K at 0.2 GPa and is consistent with the previously reported AFM transition temperature at ambient pressure for this composition [16, 28]. The transition temperatures, denoted as T^* , are defined by anomalies in the resistance behavior, corresponding to the maximum in the dR_{norm}/dT curves. At low pressures, T^* remains nearly constant up to 4.6 GPa. With further increasing pressure, T^* increases quickly near 8 GPa, coincident with the initial deviation from conventional lattice compression and the onset of the ab -plane expansion. At 8.1 GPa, the resistance data shows two pronounced features, one at 91 K, which is attributed to AFM transition following the trend from low pressures, and a second anomaly at 170 K. At higher pressures, the lower temperature feature is suppressed, whereas the anomaly at higher temperature persists up to 24.1 GPa. This change in transport behavior suggests a pressure-induced modification of the magnetic ground state. Indeed, above 8 GPa the resistance curves resemble those reported for SrCo_2P_2 in its pressure-induced FM phase [12]. The similarity suggests that FM-like behavior emerges in $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ above 8.1 GPa and the presence of two anomalies in the resistance data further suggests that $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ is in the mixed ucT and cT phase.

At face value, the XRD and transport data collected at 8.4 and 8.1 GPa, respectively, appear to be inconsistent. The x-ray data indicates the ucT phase, whereas the transport data suggests the presence

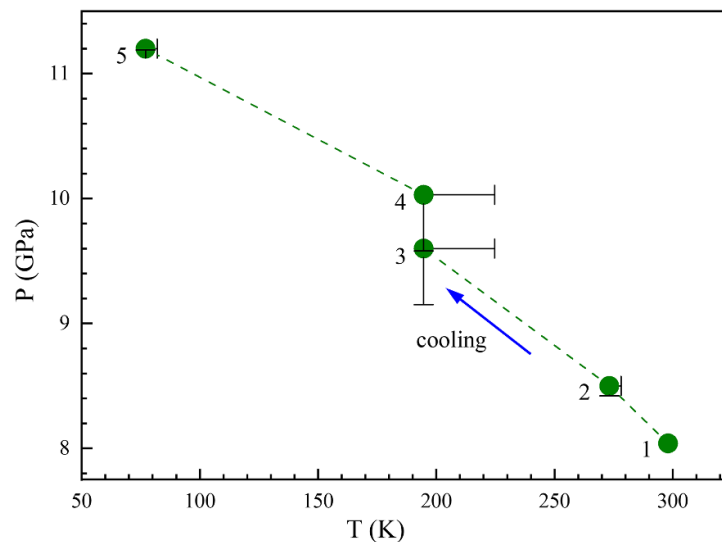


Figure 3. Pressure-temperature test in the Cu–Be DAC used in the electrical resistance experiment. Data points are labeled 1–5 based on the measurement sequence. These points were taken sequentially at room temperature (1), ice water temperature (2), dry ice temperature (3), dry ice temperature again after a brief warming (4), and liquid nitrogen temperature (5). The temperature error bars are from the temperature changes during pressure measurements and the pressure uncertainties are estimated from the corresponding temperature changes.

of the high-temperature FM-like state. It is noted that the resistance data at 8.1 GPa also shows a pronounced anomaly around 260 K. As seen in figure 2(a), 8.1 GPa lies at the onset of a rapid pressure-induced increase in resistance with pressure. Therefore, this anomaly may arise from a cooling-induced increase in the actual pressure experienced by the sample, driving the sample into the nearby cT phase. To test this possibility, a separate pressure-temperature test was performed in the same DAC as in the resistance experiment under comparable conditions, including the same gasket material, sample chamber size, and pressure medium. The results of this test are summarized in figure 3. Pressure was initially applied to 8.0 GPa at room temperature and then the cell was cooled to low temperatures (associated with ice water, dry ice, and liquid nitrogen) to monitor the corresponding pressure change. The test shows that pressure in the sample chamber can increase substantially upon cooling, likely due to differential thermal contraction among the DAC components, gasket, and pressure medium. Under the present rapid cooling conditions, the pressure increased by approximately 0.5 GPa at 273 K and by more than 3 GPa at 77 K. Although these absolute pressure values should not be taken as a direct calibration for the PPMS measurements, because the cooling rate differs significantly from the slow temperature sweep used in the PPMS, the test provides a useful reference for estimating the possible magnitude and direction of pressure drift at low temperature. It suggests that the actual low temperature pressure during the resistance measurements can easily be 1.5–2.5 GPa higher than the nominal room-temperature pressure. Thus, the anomaly near 260 K is likely not solely an intrinsic temperature-driven feature, but instead reflects the combined effect of cooling and the associated increase in sample pressure. This effect should also be considered when comparing pressure-dependent phase boundaries resulted from room-temperature XRD and low-temperature resistance experiments, especially near the ucT–cT transition region, where relatively small pressure changes can strongly influence the structural and magnetic ground states.

3.3. Discussion

The combined structural and electrical transport results are summarized in a temperature-pressure phase diagram shown in figure 4. At low pressures, $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ is in the layered tetragonal $I4/mmm$ structure with a relatively large c -lattice parameter, consistent with the ucT phase [16]. The pressure evolution of the c/a ratio provides a sensitive measure of the ucT–cT transition [1, 5, 6, 12]. As discussed above, the XRD measurements show that the first deviation from conventional compression appears at 8.4 GPa, where the in-plane lattice parameter begins to deviate from its lower pressure behavior. A decrease in c/a , together with a discontinuity in the unit cell volume, indicates the transition toward the cT phase [4, 5, 12]. At 9.7 GPa, $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ is in the mixed phase of ucT and cT. The transition is completed before 12 GPa and the structural parameters recover a more conventional pressure dependence. The pressure range between 8 and 11 GPa is shown as a mixed phase (ucT and cT) region. The

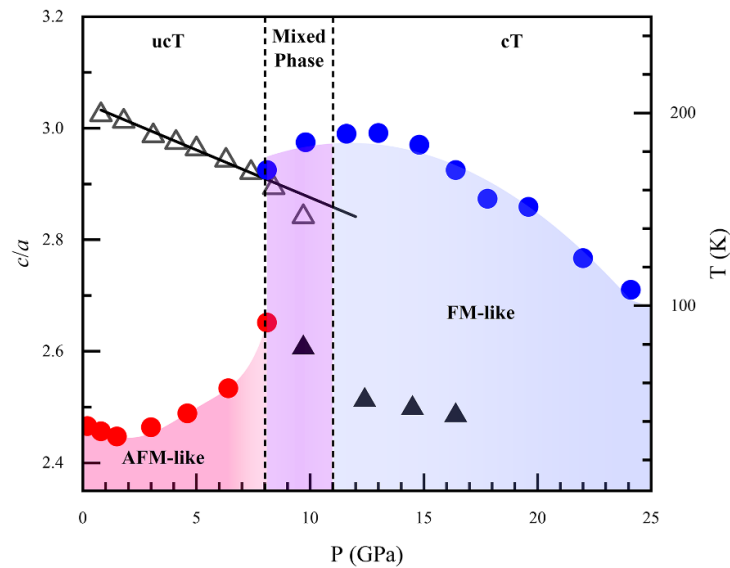


Figure 4. Proposed temperature-pressure phase diagram of $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ constructed from high-pressure XRD and electrical resistance measurements. Red and blue points represent transition temperatures determined from anomalies in dR_{norm}/dT . Gray triangles show the pressure evolution of the c/a ratio obtained from XRD data. Open and closed symbols correspond to the refined ucT and cT structural parameters, respectively. Dashed vertical lines denote approximate mixed (ucT and cT) region. The AFM-like and FM-like labels denote transport regimes inferred from resistance anomalies and comparison with related compounds, and they do not represent magnetic structures directly determined in the present measurements. The solid line through the c/a data is a guide to the eye.

resistance data suggests AFM-like behavior up to 6.4 GPa. At 8.1 GPa, two anomalies are observed in the resistance data at low temperatures, supporting a mixed AFM and FM-like state, consistent with the mixed phase concluded from the room temperature XRD data at 9.7 GPa. The difference between the transition pressures identified by the XRD and resistance experiments may be attributed in part to the fact that the XRD data were collected at room temperature, while the resistance anomalies are observed at low temperatures, causing the actual sample pressure in the low temperature resistance measurements to be higher than the pressures measured at room temperature. In addition, because the XRD and transport measurements used different pressure-transmitting media, small differences in the apparent transition pressures may also arise from differences in hydrostaticity and pressure gradients.

In figure 4, the structural data were plotted at the pressures measured during the room-temperature XRD experiment, whereas the transport transition temperatures were plotted against the nominal pressures measured by ruby fluorescence at room temperature before cooling. No numerical correction was applied to the transport pressures. Although the separate pressure-temperature test shown in figure 3 demonstrates that the pressure in the Cu–Be DAC tends to increase upon cooling, that test was performed under rapid and uncontrolled cooling conditions that differ substantially from the slow temperature sweep used in the PPMS measurements. It therefore does not provide a quantitative calibration of the pressure at the temperatures of the resistance anomalies. The test is used only to establish the likely direction of the pressure change and to show that cooling-induced pressure drift may contribute to the apparent difference between the transition pressures inferred from XRD and transport. Accordingly, the phase boundaries in figure 4 should be regarded as approximate rather than sharply determined thermodynamic boundaries.

The observed structural behavior closely resembles the pressure-induced collapse recently reported for the parent compound SrCo_2P_2 [12]. In that study, the resistance measurements were complemented by DFT calculations to discuss possible mechanisms driving the structural collapse and accompanying magnetic response. The calculations showed that the collapse is associated with strong changes in the electronic structure: P p_z antibonding states that are partially occupied below the transition shift above the Fermi level upon compression, consistent with depopulation of antibonding states and formation of interlayer P–P bonds. The calculations also indicated enhanced Co d_{xy} weight in the density of states near the Fermi level in the collapsed phase, which was linked to an itinerant FM instability. A similar bonding-driven electronic reconstruction may occur in $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$, although composition-specific DFT calculations will be required to verify this scenario. It is important to distinguish, however, between the effects of Ni/Co substitution and applied pressure. In $\text{Sr}(\text{Co}_{1-x}\text{Ni}_x)_2\text{P}_2$, Ni substitution

directly changes the band filling, whereas applied pressure primarily modifies the electronic structure indirectly through lattice compression, changes in orbital overlap, and the ucT–cT collapse.

The structural transition region coincides with pronounced changes in the characteristic temperature extracted from transport measurements. At low pressure, the resistance anomaly is consistent with previous measurements on this composition, where AFM order was reported at ambient pressure [16, 28]. Therefore, this region is labeled as AFM-like in figure 4. In the ucT phase, the transition temperature remains nearly pressure independent up to approximately 4.5 GPa, indicating that moderate compression of the uncollapsed structure has only a weak effect on the electronic or magnetic state. Above 4.5 GPa, even though the sample is still in the ucT phase and the signature of the magnetic transition is still consistent with AFM ordering, the transition temperature starts to increase dramatically. This increase in the AFM ordering temperature is interrupted by the cT transition, which is accompanied by a change to transport behavior consistent with possible FM ordering at discontinuously higher temperatures. Characteristic temperature T^* of the FM-like anomaly reaches ~ 190 K between 12 and 14 GPa and then gradually decreases to ~ 100 K by ~ 24 GPa. This behavior indicates that the electronic or magnetic response is most strongly modified within the ucT–cT transition regime, where interlayer bonding and electronic structure are expected to change rapidly.

At higher pressures, the resistance curves resemble those reported for SrCo_2P_2 in its pressure-induced FM state [12]. The high-pressure region is therefore labeled FM-like, suggesting a possible pressure-driven crossover from AFM-like to FM-like behavior in $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$. We emphasize that the present measurements do not directly measure the magnetic order parameter, such as the staggered magnetization for an AFM state or the spontaneous magnetization for an FM state. The magnetic assignments are based on the evolution of the resistance anomalies and comparison with previous studies of $\text{Sr}(\text{Co}_{1-x}\text{Ni}_x)_2\text{P}_2$ and pressure-induced ferromagnetism in SrCo_2P_2 . Consequently, the present data establish the coupling between the ucT–cT structural collapse and the crossover in transport behavior, but do not independently determine the magnetic structure or the magnitude of the ordered moment. Direct high-pressure magnetic measurements will be required to establish the nature and pressure evolution of magnetic order in the cT phase.

Several qualitative conclusions can be drawn from the combined structural and transport trends. The opposite pressure dependence of the a - and c -lattice parameters appears to play an important role in the evolution of the transport response. In chemically substituted $\text{Sr}(\text{Co}_{1-x}\text{Ni}_x)_2\text{P}_2$, increasing Ni concentration decreases c and increases a , accompanied by a change from FM order to AFM order with increasing Ni concentration [16]. Under pressure, $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ exhibits similar changes in the lattice parameters with lattice collapse, but the transport data instead suggest a change from AFM-like to FM-like behavior. This contrast indicates that the lattice collapse can not be understood solely in terms of the individual changes in a and c . Rather, the structural collapse, which is consistent with the development of interlayer $P-P$ bonding, and the associated electronic reconstruction may modify the exchange pathways, thereby changing the balance between in-plane and interlayer magnetic interactions.

4. Conclusions

The structural and resistive properties were investigated in $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$. Both data sets suggest that there is a first-order ucT to cT transition as pressure is increased beyond 10 GPa. The transition is characterized by the onset of in-plane lattice expansion, a rapid contraction of the c -axis, a discontinuity in the unit cell volume, and a large decrease in the c/a ratio between 10 and 12 GPa. Electrical resistance measurements under pressure reveal a low-pressure anomaly near the previously reported AFM transition temperature for this composition. With increasing pressure, this AFM-like feature in the resistance is first suppressed and then increases dramatically as the cT transition is approached. At the cT transition, the shape and characteristic temperature of the resistance anomaly change discontinuously, consistent with the emergence of a possible FM-like transport regime. At higher pressure, the resistance versus temperature behavior resembles the transport behavior reported for the FM state in SrCo_2P_2 . The results establish a temperature-pressure phase diagram for $\text{Sr}(\text{Co}_{0.88}\text{Ni}_{0.12})_2\text{P}_2$ and demonstrate strong coupling between ucT to cT transition and magnetic behavior. Additional high-pressure magnetic or thermodynamic measurements, such as magnetization, magnetic susceptibility, neutron diffraction, or heat capacity, as well as composition-specific DFT calculations, would be valuable for establishing the microscopic nature of the high-pressure cT state.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

The data supporting the findings of this study are available from the corresponding author upon reasonable request. The data are not publicly archived because they include specialized high-pressure diffraction and transport datasets, associated calibration files, and analysis outputs that require contextual information regarding the experimental configuration, pressure calibration, and refinement procedures for proper interpretation. The authors will provide the relevant data and supporting information to qualified researchers upon reasonable request.

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