

Role of atomic site for the phase transition in kagome lattice compounds: A case study of ScV_6Sn_6 by NMR hyperfine interactions

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(Received 18 March 2025; accepted 27 August 2025; published 15 September 2025)

Vanadium-based kagome metal of ScV_6Sn_6 has been of current interest as it features unique charge density wave (CDW) ordering accompanied by a structural phase transition, indicating the importance of lattice distortion for the onset of CDW order. To unveil the role of each individual atomic site for the phase transition, we employed a local probe through the nuclear magnetic resonance (NMR) measurements in which the NMR signals from ^{45}Sc , ^{51}V , and ^{119}Sn nuclei in both normal and CDW states were observed. From the comparison between the quadrupole splitting of ^{45}Sc and ^{51}V NMR satellite lines, a noticeable increase in the ^{45}Sc quadrupole frequency below the transition temperature was identified. The finding can be accounted for by the structural distortion mainly involving the displacement of Sc and Sn atoms along the crystal c axis. From the analysis of the temperature dependences of the NMR shift, we quantitatively obtained the change in the electronic states for each atom associated with the phase transition. In particular, we demonstrated a marked reduction in the V $3d$ density of states at the Fermi level, which can be rationalized as a manifestation of the structural transition. Remarkably, we resolved three ^{119}Sn NMR resonance lines corresponding to three nonequivalent crystallographic Sn sites and therefore estimated the variation in the $5s$ electronic states of each Sn atom in ScV_6Sn_6 .

DOI: [10.1103/81tx-2mc6](https://doi.org/10.1103/81tx-2mc6)

I. INTRODUCTION

The recently discovered kagome metal of ScV_6Sn_6 has drawn enormous interest as it undergoes a structural phase transition into unique charge density wave (CDW) order at the transition temperature $T_C \simeq 92$ K [1]. Many theoretical and experimental investigations have provided evidence that the primary mechanism for the CDW formation is the structural instability, with little effect driven by the electronic Fermi surface nesting (FSN) [2–22]. In the CDW state, the distorted structure involves a modulation of Sc and Sn atoms along the crystal c axis, while the V site is almost unchanged. The modulation leads to an intense periodic $(1/3, 1/3, 1/3)$ wave vector propagating within the ab plane, which gives rise to a long-range $\sqrt{3} \times \sqrt{3} \times 3$ CDW order. It is worthwhile mentioning that a related kagome compound of CsV_3Sb_5 simultaneously exhibits a structural distortion with CDW ordering at around 94 K in addition to the appearance of the superconductivity below 2.7 K [23]. Unlike the case of ScV_6Sn_6 , the distortion of the V-containing kagome sheet is crucial for the onset of CDW ordering in CsV_3Sb_5 [24–26]. The comparison high-

lights the key role of individual atomic site for the emergence of the CDW phase transition in various kagome systems.

Pristine ScV_6Sn_6 adopts a layered hexagonal HfFe_6Ge_6 structure type (space group $P6/mmm$) at room temperature [1]. As depicted in the inset of Fig. 1, the crystallographic structure involves five nonequivalent atoms Sc, V, Sn1, Sn2, and Sn3, corresponding to the $1a$, $6i$, $2e$, $2d$, and $2c$ sites in Wyckoff notations, respectively. There are two kagome sheets independently formed by V and Sn1 atoms. They are alternatively separated by a honeycomb layer composed of Sn2 atoms and triangular layers of Sc and Sn3 atoms. It is noteworthy that ScV_6Sn_6 is the only member showing the structural phase transition among the V-based kagome compounds in the HfFe_6Ge_6 -type family [1,2,11,27–31]. The unique phenomenon has been attributed to the small radius of the Sc atom, which gives rise to a weaker interaction within the ab plane and introduces a higher degree of freedom for the lattice relaxation along the crystal c axis [1,2,10,11]. Consequently, it results in an out-of-plane modulation of Sc and Sn1 atoms, leading to a distorted structure with a long-range CDW order below 92 K.

Nuclear magnetic resonance (NMR) is known as a site-selective tool, offering the local information of structural and electronic characteristics of the selected crystallographic site. It is thus well suited for the employment of NMR techniques on the materials with charge ordering and/or structural distortion, offering significant insights into the underlying mechanisms of the phase transition [14,32–47]. For example, the structural and electronic features of the CDW kagome

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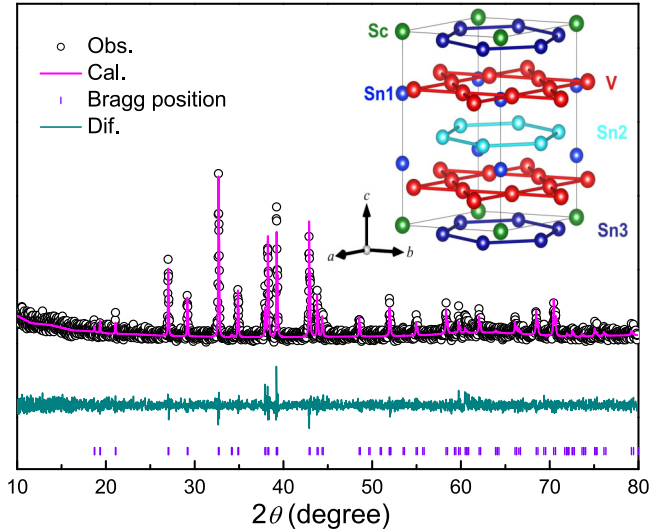


FIG. 1. Room-temperature powder X-ray diffraction (XRD) pattern with the Rietveld refinement. The black cross and magenta and dark cyan lines denote the measured data, calculated profile, and difference between the observed and calculated intensities, respectively. Inset: Crystal structure of pristine ScV_6Sn_6 .

metals AV_3Sb_5 ($A = \text{K}, \text{Rb}, \text{Cs}$) have been characterized by means of the NMR spectroscopy [42–47]. To explore the essential role of each individual atomic site for the phase transition of ScV_6Sn_6 , we carried out the NMR measurement with successfully obtaining NMR signals from ^{45}Sc , ^{51}V , and ^{119}Sn nuclei. By analyzing the quadrupole splitting of the ^{45}Sc and ^{51}V NMR satellite lines, it allows us to obtain the information of the electric field gradient (EFG) of the probed site, providing additional evidence for either site responsible for the structural distortion. From the temperature-dependent NMR shift of each crystallographic site, we unveiled the change in the electronic states for the specific atom accompanied by the CDW transition in ScV_6Sn_6 .

II. EXPERIMENT RESULTS AND DISCUSSION

Single crystals of ScV_6Sn_6 were grown by means of a self-flux method. The Sc, V, and Sn elements were mixed in a ratio of $\text{Sc}:\text{V}:\text{Sn} = 1:6:40$ and placed in an alumina crucible that was sealed in a quartz tube under partial argon pressure. The sealed tube was heated to 1100°C at a rate of $100^\circ\text{C}/\text{h}$, held at this temperature for 20 h, and then slowly cooled to 600°C with a rate of $2^\circ\text{C}/\text{h}$. All resulting ingots were etched in diluted HCl to remove residual Sn from the crystal surface. The XRD was performed using the powdered specimen obtained from crushed crystals. The XRD result with Rietveld refinement is shown in Fig. 1, yielding the lattice parameters $a = 5.476 \text{ \AA}$ and $c = 9.177 \text{ \AA}$ at room temperature, close to those reported in the previous studies [1,2,20,31].

NMR measurements were performed under a constant field of $H = 7.077 \text{ T}$. To avoid the skin depth problem of the rf transmission power, we used a powder sample by crushing the single crystals of ScV_6Sn_6 . The specimen was put in a plastic vial that showed no observable ^{45}Sc , ^{51}V , and ^{119}Sn NMR signals. For a powdered specimen, the NMR spectra appear as

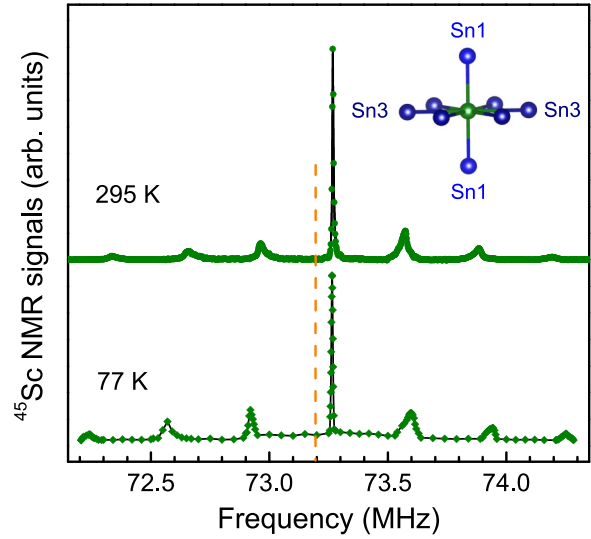


FIG. 2. Resolved ^{45}Sc NMR resonance lines of ScV_6Sn_6 measured at 295 and 77 K, respectively. The dashed vertical line denotes the position of the ^{45}Sc reference frequency. Inset: The local structure around the Sc site with neighboring Sn1 atoms in the c axis and Sn3 atoms within the ab plane.

typical powder patterns that were mapped out by integrating spin echo signals of various excitations. The NMR shift K is defined as $K = (\nu_m - \nu_R)/\nu_R$, where ν_m is the frequency position of the maximum for each spectrum and ν_R is the reference resonance frequency of the probed nucleus [48]. Here, ν_R is associated with the nuclear gyromagnetic ratio γ_n of the specific nucleus as $\nu_R = \gamma_n H / 2\pi$ with $^{45}\gamma_n = 2\pi \times 10.343 \text{ MHz T}^{-1}$ for the ^{45}Sc nucleus obtained from aqueous ScCl_3 , $^{51}\gamma_n = 2\pi \times 11.193 \text{ MHz T}^{-1}$ for the ^{51}V nucleus from aqueous VOCl_3 , and $^{119}\gamma_n = 2\pi \times 15.867 \text{ MHz T}^{-1}$ for the ^{119}Sn nucleus from aqueous $(\text{CH}_3)_4\text{Sn}$.

A. ^{45}Sc NMR

Since the crystallographic symmetry at the Sc site is not cubic in ScV_6Sn_6 , the ^{45}Sc quadrupole nucleus (nuclear spin $I = 7/2$) coupling with the EFG would lead to six NMR satellite lines in addition to the central transition line [48]. In Fig. 2, we present two representative ^{45}Sc NMR powder patterns with distinctive peak features measured at 295 and 77 K, corresponding to the high-temperature (HT) normal and low-temperature (LT) CDW phases, respectively. It is worthwhile mentioning that the observed resonance lines remain quite narrow ($\simeq 10 \text{ kHz}$) in the LT phase, giving evidence that the phase transition is not relevant to the magnetic ordering, in which an extremely broad spectrum accompanied by a large frequency shift in the NMR resonance line should take place. In principle, the electric quadrupole interaction is the major effect shaping the satellite lines, and the quadrupole frequency ν_Q can be obtained directly from the separation of these lines. From the distinct satellite peaks, which are equally spaced by $\nu_Q/2$, we determined $\nu_Q \simeq 0.61 \text{ MHz}$ at 295 K and $\simeq 0.69 \text{ MHz}$ at 77 K. The observation suggests a large increase in ν_Q from the HT to LT phases. To gain more insight into the change of ν_Q across the phase transition, we measured the first set

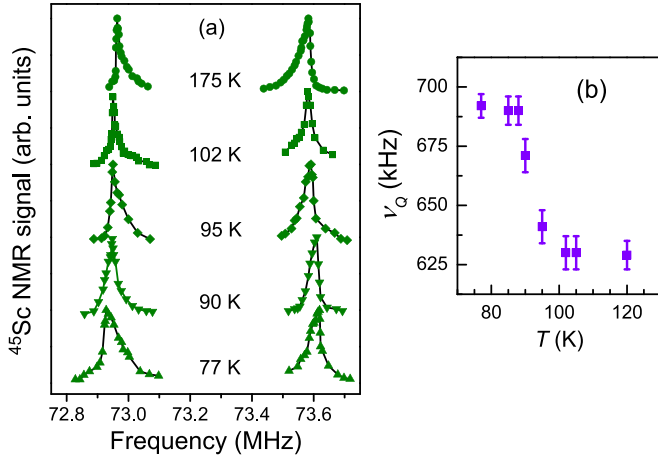


FIG. 3. (a) ^{45}Sc NMR satellite lines arising from the $\pm 1/2 \leftrightarrow \pm 2/3$ transitions measured above and below the phase transition temperature of ScV_6Sn_6 . (b) Temperature variation of ^{45}Sc ν_Q in the vicinity of T_C .

of the ^{45}Sc NMR satellite lines ($\pm 1/2 \leftrightarrow \pm 2/3$ transitions) at various temperatures, with the results displayed in Fig. 3(a). The temperature variation of ν_Q in the vicinity of T_C was thus obtained, as illustrated in Fig. 3(b). It is apparent that the value of ν_Q increases abruptly upon cooling below T_C , demonstrating a substantial enhancement of approximately 13% in the ^{45}Sc ν_Q undergoing the phase transition.

Here, ν_Q is defined by the nuclear quadrupole moment Q and the largest principle axis component of the EFG tensor of V_{zz} as $-\nu_Q = 3eQV_{zz}/[2I(I+1)h]$ (h is the Planck constant). The observed increase in ν_Q is associated with the enhancement in the EFG, which arises from the change in the noncubic arrangement of the charged lattice ions and the nonuniform charge density of the valence electrons. The former mechanism can be pictured from a local structure centered at the Sc site with nearby atoms where the neighboring Sn1 atoms, reside in the direction of the crystal c axis, while the Sn3 atoms on the ab plane, as illustrated in the inset of Fig. 2. To some extent, a sizable atomic displacement from the original position along the c axis would give rise to a marked change in the EFG around the probed site. As a matter of fact, previous XRD results revealed that Sc and Sn1 atoms displace up to $0.16 \text{ \AA}$ along the c axis below T_C [1,2,11]. It is thus likely that the major contribution to the EFG change should be from the out-of-plane structural distortion. Such a scenario is consistent with the reported results from a variety of theoretical and experimental investigations of ScV_6Sn_6 [1–4,10,11].

The temperature variation of the ^{45}Sc NMR shift ^{45}K for ScV_6Sn_6 is displayed in Fig. 4(a), showing positive shifts between 77 and 295 K. The positive values of ^{45}K have been reported in a variety of Sc-based intermetallics such as $\text{Sc}_5\text{Ir}_4\text{Si}_{10}$, ScPd_2Al , and ScSb [49–51]. Here, ^{45}K can be decomposed into three parts as $^{45}\text{K} = K_{\text{orb}} + K_s + K_d$. The first term K_{orb} is the orbital shift, arising from the orbital magnetic moment of electrons induced by the applied field. Typically, K_{orb} is independent of or weakly dependent on temperature. The second one K_s is the s -contact Knight shift, which is proportional to the s -character Fermi-level density of states

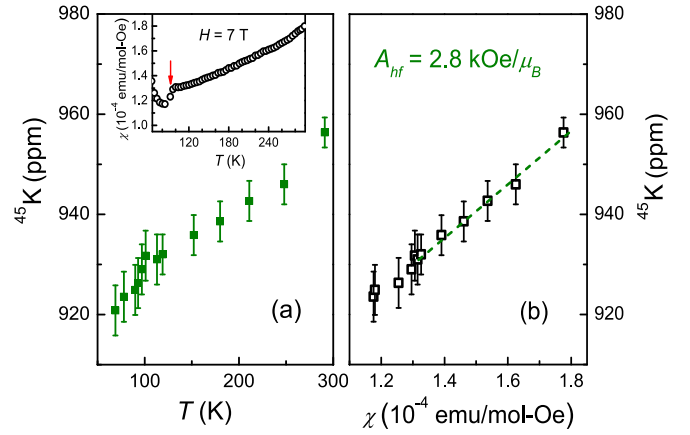


FIG. 4. (a) Temperature dependence of the ^{45}Sc NMR shift ^{45}K for ScV_6Sn_6 . Inset: Temperature variation of the magnetic susceptibility χ measured under a constant field of 7 T. A sudden drop at T_C was marked by an arrow. (b) A plot of ^{45}K vs χ of ScV_6Sn_6 . The dashed line indicates the linear behavior above T_C .

(DOS) $N_s(E_F)$ in conventional metals. The third term K_d is the d -spin shift, which involves the spin polarization of the closed shells and the s -character electrons in the conduction bands via d electrons. Note that the sign of K_d is negative, owing to the antiparallel orientation between core spins and the unpaired spins responsible for the polarization [48]. In the normal state, ^{45}K gradually decreases upon lowering temperature, similar to the feature found in the bulk magnetic susceptibility χ shown in the inset of Fig. 4(a). In principle, the relationship between the observed NMR shift K_{obs} and χ can be correlated as

$$K_{\text{obs}}(T) = K_o + \frac{A_{\text{hf}}}{N_A} \chi. \quad (1)$$

Here, K_o is the temperature-independent shift, N_A is the Avogadro constant, and A_{hf} is the hyperfine coupling constant arising from a combination of hyperfine interactions sensed by the probed nucleus. In Fig. 4(b), we provided the Clogston-Jaccarino plot that shows the relation between ^{45}K and χ with temperature as the implicit parameter [52]. To avoid any field-dependent effect, the χ measurement was performed under a field of 7 T, close to the field used in our NMR experiment. The linear behavior, demonstrated by a straight line, indicates a unique hyperfine coupling constant in the HT phase. From the slope of the line, we extracted $A_{\text{hf}} = 2.8 \pm 0.5 \text{ kOe}/\mu_B$ (μ_B is the Bohr magneton) for the Sc site of ScV_6Sn_6 . The positive value of A_{hf} signifies that the temperature-dependent ^{45}K above T_C is mostly related to the Sc $3s$ electrons since the Sc $3d$ core-polarization hyperfine interaction would give rise to an opposite contribution to A_{hf} .

In the vicinity of T_C , a minor fall of about 10 ppm in ^{45}K was found, indicative of little change in the electronic states at the Fermi surfaces, being consistent with the viewpoint from theoretical calculations [10]. While the Sc $3d$ partial Fermi-level DOS $N_d(E_F)$ is higher than $N_s(E_F)$ in ScV_6Sn_6 [4,10,17–19], the observation cannot be purely accounted for by a decrease in $N_d(E_F)$ since the direction of polarization by $3d$ orbitals would cause an increase in ^{45}K , opposite to the observed feature. As a matter of fact, the Sc $3s$ hyperfine

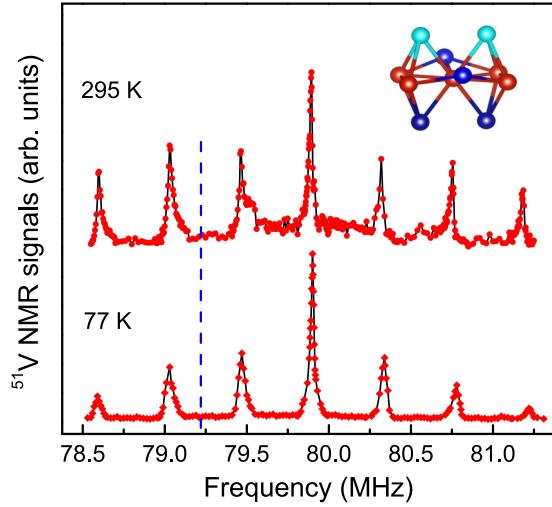


FIG. 5. Resolved ^{51}V NMR resonance lines of ScV_6Sn_6 obtained at 295 and 77 K, respectively. The dashed vertical line denotes the position of the ^{51}V reference frequency. Inset: The local structure around the V site with surrounding atoms.

field is approximately 10 times larger than the Sc 3d core-polarization hyperfine field [53], and therefore a limited loss of Sc 3s electronic DOS at the Fermi level could give rise to a non-negligible reduction in ^{45}K . Thus, it is likely that a decrease in $N_s(E_F)$ would significantly offset the contribution from the reduction in $N_d(E_F)$, leading to a tiny drop in ^{45}K at around T_C .

B. ^{51}V NMR

Figure 5 shows two ^{51}V NMR powder patterns of ScV_6Sn_6 measured at 295 and 77 K, respectively. For the ^{51}V nucleus with nuclear spin $I = 7/2$, the single crystallographic V site in the HT phase of ScV_6Sn_6 yields six NMR satellite lines due to the quadrupole coupling within a noncubic electric environment. The steric interactions can be clearly viewed from a local structure around the V site with neighboring atoms, as depicted in the inset of Fig. 5. In the LT phase, three nonequivalent crystallographic V sites induced by structural distortions should give rise to three sets of resonance lines as recently observed by orienting the crystalline sample with the external field [14]. We, however, failed to resolve the three sets of quadrupole splitting of the satellite lines, presumably due to the use of unaligned specimens in our NMR experiment. In fact, Guehne *et al.* have determined ^{51}V $\nu_Q = 0.475$ MHz with the asymmetry parameter of EFG $\eta \simeq 0.83$ above T_C [14]. Also, $\nu_Q = 0.463, 0.489$, and 0.499 MHz with $\eta \simeq 0.91, 0.81, 0.78$ for the corresponding V site below T_C have been extracted. Since the variations of ν_Q and η are small in the LT phase, it is likely that the ^{51}V NMR powder pattern would appear as a set of broadening lines. Accordingly, our ^{51}V NMR spectrum at 77 K is a superposition of the results from three nonequivalent V sites, and the obtained ν_Q is an averaged value of the three V sites. From the estimated $\nu_Q \simeq 0.43$ MHz at 295 K and $\simeq 0.44$ MHz at 77 K, it is clear that the increase in the $^{51}\text{V}\nu_Q$ is much weaker than the observed enhancement of approximately 13% in the $^{45}\text{Sc}\nu_Q$. Therefore,

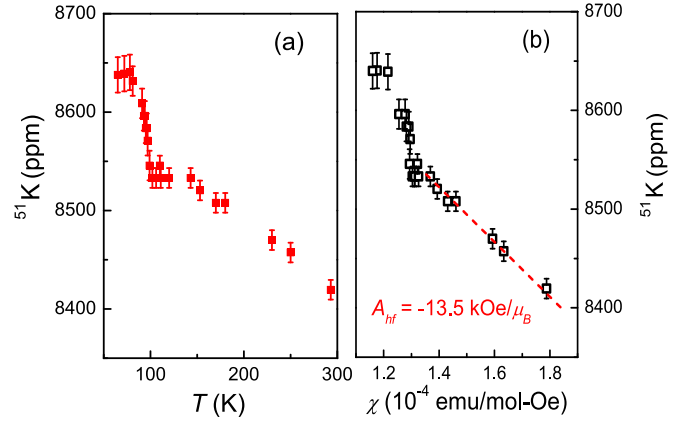


FIG. 6. (a) Temperature dependence of the ^{51}V NMR shift ^{51}K for ScV_6Sn_6 . (b) A plot of ^{51}K vs χ of ScV_6Sn_6 . The dashed line indicates the linear behavior above T_C .

by comparing the changes of the NMR quadrupole splitting at the V and Sc sites, we pointed out that the EFG around each V site has a marginal change, while the Sc site shows a substantial increase undergoing the structural phase transition.

The temperature dependence of the ^{51}V NMR shift ^{51}K is displayed in Fig. 6(a), showing positive shifts within the temperature range we measured. The large positive ^{51}K is consistent with the recently reported values of 6000–8000 ppm, mainly due to the ^{51}V orbital shift $^{51}\text{K}_{\text{orb}}$ [14]. The dominant contribution from $^{51}\text{K}_{\text{orb}}$ has been observed in various V-based intermetallics such as kagome metals of CsV_3Sb_5 and RbV_3Sb_5 [42–46] and Heusler alloys of Fe_2VAl and Fe_2VGa [54–57]. In the normal state, ^{51}K gradually increases upon lowering temperature, opposite to the trend of χ . The plot of ^{51}K against χ indicates linear behavior, as demonstrated by a dashed line in Fig. 6(b). We thus extracted $A_{\text{hf}} = -13.5 \pm 0.7 \text{ kOe}/\mu_B$ for the V site of ScV_6Sn_6 from the slope of the line according to Eq. (1). The obtained negative A_{hf} gives a confirmation that the temperature-dependent ^{51}K is governed by the V 3d core-polarization hyperfine coupling.

Near T_C , we observed a sudden jump in ^{51}K , which is related to the abrupt change in V 3d Fermi-level DOS $N_d(E_F)$. Within the picture of the noninteracting electrons for ScV_6Sn_6 , the magnitude of $N_d(E_F)$ can be evaluated from the relationship as $^{51}\text{K} = \mu_B H_{\text{hf}}^d N_d(E_F)$. Here, H_{hf}^d is the V 3d core-polarization hyperfine field and the unit of $N_d(E_F)$ is states eV^{-1} per V atom. From an observed increase of about 110 ppm in ^{51}K and the calculated value of $H_{\text{hf}}^d = -117 \text{ kOe}$ for the V-based metals [54], we estimated a decrease in $N_d(E_F) \simeq 0.15$ states eV^{-1} per V atom, which corresponds to a sizable reduction in the 3d Fermi-level DOS of 0.9 states $\text{eV}^{-1} \text{ f.u.}^{-1}$. Therefore, the sudden fall in χ during the phase transition can be accounted for by the profound modification in the V 3d band structure. Our finding is also consistent with the observation of the ^{51}V NMR spin-lattice relaxation rate $1/T_1$, where the determined Korringa constant $1/T_1 T$ was found to drop by a factor of 2 below T_C [14]. Since the Korringa constant is proportional to the square of $N_d(E_F)$ for nonmagnetic metals [58], the analysis of ^{51}V NMR $1/T_1$ yielded a loss of 3d DOS of approximately 30% during the phase transition [14]. Nevertheless, the electronic

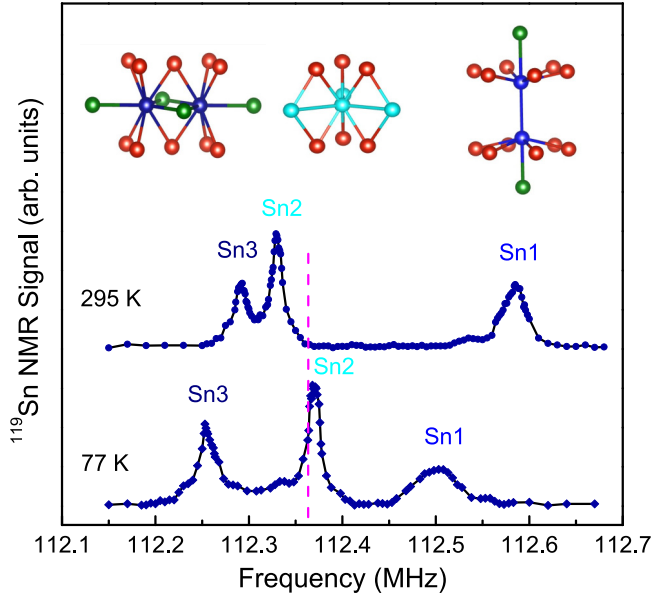


FIG. 7. Three resolved ^{119}Sn NMR resonance lines of ScV_6Sn_6 measured at 295 and 77 K, respectively. The dashed vertical line denotes the position of the ^{119}Sn reference frequency. The insets illustrate the local structures around the Sn1, Sn2, and Sn3 sites, respectively.

band reconstruction is unlikely to result from the FSN as excluded by the optical conductivity measurement, which indicated the lack of the signature of the CDW gap formation [5]. Hence, the reduction in $N_d(E_F)$ obtained from our analysis of ^{51}K is essentially a manifestation of the structural transition in ScV_6Sn_6 .

C. ^{119}Sn NMR

For the ^{119}Sn nucleus with nuclear spin $I = 1/2$, there is no quadrupole coupling and only a central transition line is observed for each crystallographic Sn site. In Fig. 7, we present two sets of the ^{119}Sn NMR powder patterns of ScV_6Sn_6 taken at 295 and 77 K, respectively. Each spectrum features three ^{119}Sn NMR resonance peaks corresponding to three nonequivalent crystallographic Sn sites. The site identification is given by virtue of the different change of the ^{119}Sn NMR shift ^{119}K across T_C , as shown in Fig. 8. The scenario is related to the neighboring hyperfine coupling of the probed Sn site, which is illustrated from the local structures around the Sn1, Sn2, and Sn3 sites, as depicted in the inset of Fig. 7. Among the three Sn sites in ScV_6Sn_6 , the largest change in the electronic states along with the phase transition was proposed to take place at the Sn1 site [3, 10, 11, 17–19]. Therefore, the resonance line at the highest frequency that exhibits a drastic fall in ^{119}K across T_C is attributed to the Sn1 site. Since the least impact affected by the phase transition is expected for the Sn2 site, it is reasonable to associate the marginal change in ^{119}K at around T_C with this site. Hence, the resonance line that peaks in the middle of the ^{119}Sn NMR spectrum is assigned to the Sn2 site. The remaining one featuring a peak at the lowest frequency is connected to the Sn3 site.

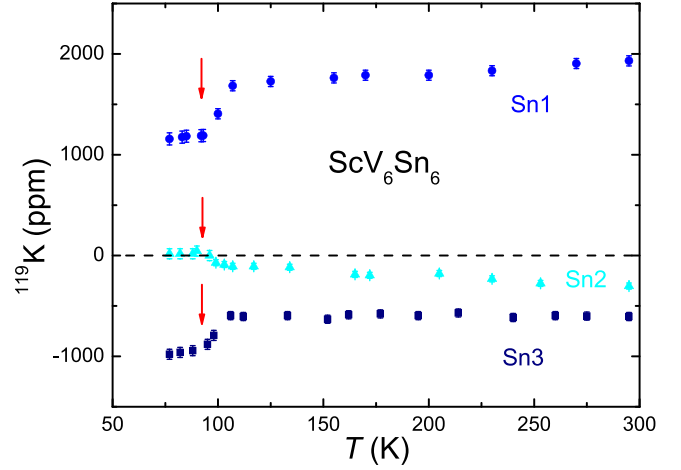


FIG. 8. Temperature variations of the ^{119}Sn NMR shift ^{119}K for the Sn1, Sn2, and Sn3 sites of ScV_6Sn_6 measured during a warming process. The position of T_C was marked by an arrow for each Sn site. The horizontal line was drawn to denote the zero ^{119}K .

The obtained ^{119}K here is a combination of three components as $^{119}\text{K} = K_{\text{orb}} + K_s + K_{\text{tr}}$. The mechanisms for the orbital shift K_{orb} and s -contact Knight shift K_s have been described in the subsections of ^{45}Sc and ^{51}V NMR. The third term K_{tr} reflects the d electronic behavior of the neighboring atoms through the transferred hyperfine interaction via conduction electrons. Note that the transferred hyperfine interaction could cause either positive or negative K_{tr} depending on the direction of polarization by the transferred hyperfine field. In spite of the fact that the electronic states of Sn atoms are dominated by p orbitals near the Fermi level, the effect arising from p electrons on ^{119}K should be neglected, owing to the relatively weak core polarization from p orbitals [37–39, 48].

Figure 8 displays the temperature dependence of ^{119}K for each individual Sn site measured during a warming process. In the normal state, the observed ^{119}K for these three Sn sites exhibit weak dependence on temperature. In the vicinity of T_C , the decreases in $^{119}\text{K} \simeq 500$ and 350 ppm were extracted for the Sn1 and Sn3 sites, respectively. However, a small increase of about 70 ppm was obtained for the Sn2 site. Since the hyperfine field due to Sn $5s$ electrons is approximately two orders larger than that from the $5p$ core polarization [48], it is realistic to associate the abrupt drop in ^{119}K with a loss of $5s$ electrons for both Sn1 and Sn3 atoms. In contrast, the slight increase in ^{119}K for the Sn2 site could be due to a limited enhancement in the $5s$ DOS caused by the phase transition. Accordingly, from the observed changes in ^{119}K at around T_C and the calculated value of $H_{\text{hf}}^s = 1.28 \times 10^4$ kOe for the Sn $5s$ hyperfine field [48], we evaluated the decreases in $N_s(E_F) \simeq 0.013$ and $\simeq 0.01$ states $\text{eV}^{-1} \text{f.u.}^{-1}$ for the Sn1 and Sn3 atoms, respectively. Likewise, a weak increase in $N_s(E_F) \simeq 0.002$ states $\text{eV}^{-1} \text{f.u.}^{-1}$ was estimated for the Sn2 atom. Therefore, by analyzing the ^{119}Sn NMR shift of the selected Sn site, we unveiled the change of the electronic state for each individual Sn atom undergoing the phase transition.

III. CONCLUSIONS

In conclusion, we have painted a concise picture of NMR characteristics for ScV_6Sn_6 , giving a microscopic viewpoint for the change of the structural and electronic features in the vicinity of T_C . From the observation of a marked increase in the ^{45}Sc NMR quadrupole frequency below T_C , we provided concrete evidence that the lattice distortion in the CDW state is significantly associated with the large atomic displacements of the Sc and Sn1 atoms. From the drastic change in the ^{51}V NMR shift at T_C , we estimated a decrease in the V $3d$ Fermi-level DOS of about 0.9 states $\text{eV}^{-1}\text{f.u.}^{-1}$, which is mainly accounted for by the structural phase transition in ScV_6Sn_6 . In addition, we resolved three ^{119}Sn NMR resonance lines and selectively examined the change in the $5s$ electronic states of each individual Sn atom in ScV_6Sn_6 accompanied by the phase transition.

ACKNOWLEDGMENTS

This work is supported by the National Science and Technology Council (NSTC) of Taiwan under Grants No. 113-2112-M-006-024, No. 114-2112-M-006-011, No. 114-2124-M-006-004, and No. 114-2124-M-006-005. We acknowledge Dr. M. K. Lee for the magnetic susceptibility measurement. We thank Ms. S. Y. Sun for the help with performing the NMR measurement at the Core Facility Center under Grant No. 113-2740-M-006-002.

DATA AVAILABILITY

The data supporting this study's findings are available within the article.

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