Chemical and hydrostatic pressure effect on charge density waves of SmNiC$_2$

Jae Nyeong Kim$^1$, Changhoon Lee$^1$ and Ji-Hoon Shim$^{1,2,3,4}$

$^1$ Department of Chemistry, Pohang University of Science and Technology, Pohang 790-784, Korea
$^2$ Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea
$^3$ Division of Advanced Nuclear Engineering, Pohang University of Science and Technology, Pohang 790-784, Korea
E-mail: jhshim@postech.ac.kr

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Abstract. Using a first-principles density functional theory method, we have investigated the chemical and the hydrostatic pressure effects on the charge density wave (CDW) properties of the quasi-one-dimensional (1D) compound SmNiC$_2$. With increasing pressure, the relative 1D anisotropy of the electronic structure along $a$ direction is enhanced because of its Ni chain structures. From the analysis of the Fermi surface and the generalized susceptibility, we also find that the Fermi surface nesting is enhanced along the modulation vector $q_1 = (0.5, 0.52, 0)$ but is suppressed along $q_R = (0.5, 0.5, 0.5)$ under pressure. The enhancement of 1D anisotropy of SmNiC$_2$ under pressure is responsible for increasing CDW strength along $q_1$. We suggest that this quantitative analysis could be used for analysis of the pressure effect on CDW materials.

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$^4$ Author to whom any correspondence should be addressed.

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1. Introduction

SmNiC$_2$, one of the RNiC$_2$ (R: rare earth atom) compounds, has an orthorhombic CeNiC$_2$ type structure (space group 38, $Amm2$) [1–6]. It contains Ni and Sm one-dimensional (1D) chains along $a$ direction, as shown in figure 1(a). Such chains are connected with a zig-zag shape along diagonal directions. As a result, each Ni(Sm) chain is surrounded by three Sm(Ni) chains with a trigonal prism shape. C–C dimers locate between prisms to make a three-dimensional (3D) bulk network.

This compound shows the competition between the charge density wave (CDW) and ferromagnetism (FM) [1–8]. Its CDW phase is developed below $T_{CDW} = 148$ K and it completely disappears at $T_C = 17.5$ K with the FM transition. At the CDW transition, resistivity shows a sharp inflection by opening the band gap [3, 4]. From the x-ray diffraction experiment, the satellite peaks appear below $T_{CDW}$ along two independent vectors by the lattice modulation: one dominant CDW peak at $q_1 = (0.5, 0.52, 0)$ and another weak CDW peak at $q_R = (0.5, 0.5, 0.5)$ [4]. This CDW phase is interpreted as commensurate with lattice modulation of Ni chains along $a$ direction, but the frustrated 3D inter-chain coupling leads to the incommensurability along $b$ direction [5]. Theoretical band structure calculation captures the origin of the CDW phase from Fermi surface (FS) nesting [9]. Temperature dependent thermal diffuse scattering pattern shows a Kohn anomaly, which indicates the suppression in the phonon frequency along $q_1$ and $q_R$ vector by the CDW transition [4]. A high-resolution photoemission spectroscopy experiment shows the imperfect FS nesting feature by the opening of pseudo-gap below $T_{CDW}$ [7]. Below $T_C$, the local magnetic moment of Sm 4f orbital is large enough to modify the electronic structure and eventually destruct the nesting condition [4, 6]. The CDW phase could be switched to an FM phase under magnetic field near $T_C$; therefore, this compound has a potential as a spintronic device with a giant magneto resistance [6].

Under pressure, SmNiC$_2$ also has several interesting phenomena. According to a recent report of the transport properties of SmNiC$_2$, $T_{CDW}$ increases with pressure, unlike typical CDW materials. In addition, another CDW transition occurs at lower temperature ($T_{CDW2}$), which decreases with pressure [8]. This is also observed by the chemical pressure with other RNiC$_2$ systems (NdNiC$_2$ and GdNiC$_2$) [3]. However, there has been little understanding of
this phenomena. Within the CDW phase, a FM quantum criticality has been observed with the pressure near 3.8 GPa [8]. Near the quantum criticality, a variety of magnetic phases comes out and shows the interplay with the CDW phase. Although such complicated magnetic phases have also been observed in other RNiC$_2$, [10–14] the FM quantum criticality is a unique property of SmNiC$_2$.

Pressure is an important parameter for the control of not only the CDW phase but also magnetism or superconductivity. In particular, there have been many pressure experiments for transition metal chalcogenides [15–17] and some rare earth compounds [18–20], including SmNiC$_2$ [8], in order to investigate the competition between the CDW and magnetism or superconductivity. However, there has been little theoretical analysis to verify the competition mechanism and pressure dependent order parameter changes.

In this paper, the pressure effect on the electronic structure of quasi 1D SmNiC$_2$ has been investigated by using a first-principles density functional theory (DFT) method. The electronic band structures and the electrical conductivity show that SmNiC$_2$ is an electrically quasi 1D system with Ni chains along $a$ direction. Under chemical or hydrostatic pressure, relative 1D anisotropy increases mainly due to the fact that the lattice constant along the Ni chain direction suppresses. By using the calculation of the FSs and the generalized susceptibility ($\chi_0(q)$), we reveal that the CDW along $q_1$ vector is enhanced under pressure with increasing 1D anisotropy, while the CDW along $q_R$ is suppressed.
Table 1. The calculated lattice parameters of GdNiC$_2$, NdNiC$_2$ and pressurized SmNiC$_2$, compared with experimental lattice parameter of SmNiC$_2$.

| Compounds     | Pressure (GPa) | a (Å)   | b (Å)   | c (Å)   |
|---------------|----------------|---------|---------|---------|
| GdNiC$_2$     | 0              | 3.665   | 4.533   | 6.046   |
|               | −6             | 4.063   | 4.688   | 6.314   |
|               | 0              | 3.754   | 4.545   | 6.085   |
|               | 4              | 3.725   | 4.532   | 6.065   |
| NdNiC$_2$     | 0              | 3.847   | 4.555   | 6.121   |
|               | −6             | 4.063   | 4.688   | 6.314   |
|               | 0              | 3.754   | 4.545   | 6.085   |
|               | 4              | 3.725   | 4.532   | 6.065   |
| SmNiC$_2$     | 8              | 3.698   | 4.519   | 6.047   |
|               | 12             | 3.673   | 4.508   | 6.029   |
| Experiment [2] |                | 3.703   | 4.529   | 6.098   |

2. Method

To find the optimized crystal structure (both lattice constants and atomic positions) of RNiC$_2$ (R=Nd, Sm, Gd), Vienna ab initio simulation package (VASP) is used [21]. Because the aim of this work is describing FS nesting at high temperature, we consider the crystal structure with perfectly localized 4f orbital. To achieve the aim of our study, we have chosen a pseudo-potential that contains non-f orbital. The projector augmented wave method with the PBE-GGA is used for the DFT calculation [22]. The cut-off energy in the plane-wave expansion of the valence states is set to 500 eV. The $15 \times 15 \times 15$ Monkhost-pack $k$ mesh is used in the full Brillouin zone (BZ). With the total energy of each volume (−8% to +4% changes from the optimized volume), a Birch–Murnaghan equation of state is used to estimate the pressure for corresponding volume [23, 24]. Table 1 shows the lattice parameters of SmNiC$_2$ form −6 to 12 GPa and those of GdNiC$_2$ and NdNiC$_2$ at ambient pressure.

Since 4f states are treated as a core state in VASP, a WIEN2k package was used for calculating the electronic and magnetic structures of RNiC$_2$ to describe the 4f orbital of rare earth atoms more precisely [25]. This package uses a full potential L/APW + lo methods based on the DFT. As the non-overlapping radius of muffin-tin, 2.5 (rare earth), 1.95 (Ni), 1.28 (C) in atomic unit were used. The $10 \times 10 \times 10$ mesh is used for the self-consistent charge density calculation. We consider a dense $k$-mesh for precise description of the conductivity [26] ($36 \times 37 \times 37$ $k$-mesh) and the $\chi_0(q)$ ($100 \times 100 \times 100$ $k$-mesh). In the description of high temperature non-magnetic (NM) phase, a 4f orbital was treated as core state by the open-core method [25]. In the low temperature FM calculation, a GGA+U+SO ($U_{\text{eff}} = 8$ eV) method was used in order to consider the on-site Coulomb interaction ($U$) and the spin–orbit (SO) interaction.

The generalized susceptibility (Lindhard response function) $\chi_0(q)$ is calculated directly from the energy eigenvalue using

$$\chi_0(q, \omega) = \frac{1}{N} \sum_{n,n',k} \frac{f(\epsilon_{n',k+q})[1 - f(\epsilon_{n,k})]}{\epsilon_{n',k+q} - \epsilon_{n,k} - \omega + i\delta},$$

(1)
where \( f(\varepsilon) \) is the Fermi–Dirac distribution function, and \( \varepsilon_{n,k} \) and \( \varepsilon_{n',k+q} \) are the energy eigenvalues in the first BZ with band indices \( n \) and \( n' \). Because the purpose of this work is to examine the static FS nesting feature, \( \omega \) was set to 0. The real part of \( \chi_0(q) \) was taken for the description of the FS nesting strength [9, 27, 28]. We have only considered the bands which cross the Fermi level because these bands have a main contribution to \( \chi_0(q) \) and the others have featureless contribution to \( \chi_0(q) \). In equation (1) we have employed the approximation of constant matrix element. Although it cannot describe the detail strength of the FS nesting correctly, it is very useful to check the size of the FS nesting vector. Indeed, our calculation correctly captures the CDW vectors measured in experiment. There are severe numerical problems in obtaining an exact value of \( \chi_0(q) \) due to the singular value in the denominator. To solve this problem, one can use imaginary part of \( \chi_0(q) \) and sizable \( \delta \) for the broadening effect [27, 28]. Instead, we set \( \delta = 0 \) and averaged \( \chi_0(q) \) using large number of random \( k \)-points (\( \sim 10^9 \)) where the eigenvalue of the each random \( k \)-point is obtained by linear interpolation of eigenvalues from \( 100 \times 100 \times 100 \) \( k \)-mesh in the full BZ. We have confirmed that this produces a more precise function of \( \chi_0(q) \).

3. Results and discussion

The CDW is a periodic charge and lattice modulation that can be realized when the electron–phonon interaction induces an energy gap, overcoming the lattice strain energy [29, 30]. The CDW vector (2\( k_F \)) of a metallic system can usually be identified by inspecting the FS nesting, which can be understood as the realization of quasi 1D system showing Peierls instability [31]. Pressure is an important factor to control the FS nesting and the strength of the CDW phase. As pressure increases, the weaker nesting condition in system usually leads to the destruction of the CDW phase. In some cases, however, the CDW phase could be enhanced by the anisotropic lattice modulations [16, 32–34]. There is little theoretical explanation on the mechanism of enhancing CDW strength. We show that the enhancement of the CDW strength with the pressure effect on SmNiC\(_2\) by the calculation of crystal structure changes, the electronic structures, the FSs and the generalized susceptibility \( \chi_0(q) \).

3.1. Crystal structures

Figure 1(b) indicates the volume dependent lattice constants of SmNiC\(_2\) in NM phase. For comparison to NdNiC\(_2\) of larger lattice constant, we also consider the negative hydrostatic pressure (expanded volume) of SmNiC\(_2\). Under hydrostatic (lines) and chemical (open circles) pressure, the lattice constant \( a \) is more suppressed than other lattice constants because the rigid C–C dimers resist the suppression of the lattice along \( b \) and \( c \) directions. The enhancement of interatomic interactions from a shrinking lattice constant \( a \) on SmNiC\(_2\) could be related to a change of the CDW phase since the Ni chain along that direction is experimentally reported to have main contribution on the CDW phase [5]. The calculated lattice constants of other RNiC\(_2\) (R=Gd, Nd), denoted by open circles, are roughly consistent with pressurized SmNiC\(_2\) with corresponding volume. Thus, the chemical pressure on SmNiC\(_2\) shows a similar effect to the hydrostatic pressure. Note that the chemical pressure should be more responsible for enhancement of interatomic interactions due to the faster suppression of the lattice constant \( a \) (see the black open circle in figure 1(b)).
3.2. Electronic structures

Figures 2 and 3 show the electronic structures of SmNiC$_2$ at the ambient pressure for NM and FM phase, respectively. Analysis of the density of states (DOS) and band structure leads to the following observations.

(a) SmNiC$_2$ can be described as a Sm$^{3+}$Ni$^{3-}$ (C$_2$)$_0$ and the 3d block of Ni$^{3-}$ ion is almost filled with ten electrons and Sm$^{3+}$ ion have five unpaired 4f electrons. The finite band width of Sm 5d and Ni 3d orbitals in the solid makes SmNiC$_2$ metallic state (see figure 2(a)). The magnetic moment of SmNiC$_2$ is mainly developed from Sm 4f electrons because Ni 3d orbital is fully filled. The sharp DOS of Sm atom for the majority spin in figure 3(a) is contributed from 4f electron of Sm atom. The positions of the remaining minority spin 4f
The calculated band dispersion as shown in figures 2 and 3. The quasi 1D property of the electronic structure could be analyzed more quantitatively using the calculation of the electrical conductivity for each direction. Figure 3. (a) The DOS and (b) the band structures of SmNiC2 obtained by GGA+U+SO ($U_{Sm} = 8$ eV) calculation for FM phase. (a) Positive and negative DOSs indicate their contribution from majority spin and minority spin of SmNiC2. (b) The bands of Sm 5d orbitals are split near the Fermi level by the spin-exchange interaction.

The calculated magnetic moment ($\mathbf{J} = \mathbf{S} - \mathbf{L} = m_S - m_L$, where $J$, $S$, $L$, $m_S$ and $m_L$ indicate total, spin, orbital angular moment, azimuthal spin and orbital moment) is $3.01 \mu_B$ for the FM state. Due to the hybridization between the Ni 3d and Sm 4f block, the band splitting of $\approx 0.2$ eV is found near the Fermi level, as shown in figure 3(b).

(b) The calculated band dispersion as shown in figures 2 and 3(b) show band crossings at the Fermi level, mainly along $a$ direction, namely $\Gamma-X$, $S^*-Y^*$ and $U^*-Z^*$ lines. For this reason, quasi 1D electronic structures of SmNiC2 along $a$ direction is expected. In particular, the Ni 3d orbital has a dominant contribution along $\Gamma-X$ lines. The Ni atom is located in the center of the Sm trigonal prism. In general, the crystal split pattern of trigonal prism is $(d_{xy}, d_{x^2-y^2}) < d_{z^2} < (d_{xz}, d_{yz})$. However the shape of SmNi prism is distorted from a perfect triangle prism and is pressed along $c$ direction, which is higher the $d_{yz}$ orbital (along $a$ direction) above $d_{xz}$, $d_{z^2}$ orbital, leading to the split pattern $((d_{xy}, d_{x^2-y^2}) < d_{xz} < d_{z^2} < d_{yz})$. The $d_{yz}$ orbital crosses the Fermi level.

The quasi 1D property of the electronic structure could be analyzed more quantitatively using the calculation of the electrical conductivity for each direction. Figure 2(c) shows the relative electrical conductivity, calculated by the Boltzmann transport equation [26], as a function of pressure. At the ambient pressure, it shows quite an anisotropic resistivity with $\sigma_c/\sigma_a \approx 0.24(\rho_c/\rho_a \approx 4.18)$, $\sigma_b/\sigma_a \approx 0.36(\rho_b/\rho_a \approx 2.81)$. This is well matched with both our band structure analysis and the experimental results [4].

We also explore the change of the electrical properties under the chemical and hydrostatic pressure (see figure 2(c)). Under chemical pressure, denoted by open circles, electric anisotropy is enhanced from the reduction of both $\sigma_b/\sigma_a$ and $\sigma_c/\sigma_a$. However, under hydrostatic pressure (line) the $\sigma_b/\sigma_a$ ratio is decreased while the $\sigma_c/\sigma_a$ ratio is increased. The increase of conductivity

\[ \sigma_b/\sigma_a \]

\[ \sigma_c/\sigma_a \]

Each brillouin zone symbol means $\Gamma = (0, 0, 0)$, $R = (0.5, 0.5, 0.5)$, $R^* = (0.5, 1, 1)$, $S = (0.5, 0.5, 0)$, $S^* = (0.5, 1, 0)$, $T = (0.5, 0.5, 0.5)$, $T^* = (1, 0, 1)$, $U = (0, 0.5, 0.5)$, $U^* = (0, 1, 1)$, $X = (0.5, 0, 0)$, $Y = (0, 0.5, 0)$, $Y^* = (0, 1, 0)$, $Z = (0, 0, 0.5)$ and $Z^* = (0, 0, 1)$ in the reciprocal space.

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along \(c\) direction for the hydrostatic pressure could be caused by a rare earth 5d orbital. Since the atomic size of rare earth atoms decreases by chemical pressure, the overlap between rare earth 5d orbitals perpendicular to \(a\) direction is reduced, despite the shortened lattice constants. Also, the most important orbital for the CDW phase is the Ni 3d orbital \[5\] and the contribution of rare earth 5d orbital is negligible to develop the CDW phase. In the following two sections, we will discuss if the pressure behaviors of CDW phase are similar to both chemical and hydrostatic cases. This is responsible for increasing quasi 1D property of Ni chain.

3.3. Fermi surfaces

In connection with the electrical properties, we have analyzed the CDW phase in terms of the calculated FSs and \(\chi_0(q)\). As shown in figure 4(a), the two parallel FSs along \(a^*\) direction show quasi 1D behavior consistent with the electrical properties. Figures 4(b) and (c) show the two-dimensional (2D) cross sections of the FS (black) in the NM phase. The strong FS nesting is found with wave vectors \(q_1 = (0.5, 0.52, 0)\) and \(q_R = (0.5, 0.5, 0.5)\), which correspond to the experimental CDW vector (blue arrow) \[4\]. The FS nesting occurs mainly near the central part of BZ around \(\Gamma–X\) symmetry line, where the Ni 3d orbital gives a dominant contribution (see figure 2(b)). For detailed analysis of the nesting directions, the calculation of \(\chi_0(q)\) is needed.

For the FS of the FM phase, as we mentioned above, there occurred a band splitting near the Fermi level. This small band splitting leads to split FSs (red), depending on the different spin characters, as shown in figure 4. Although the split FSs looks still well nested, like the NM phase, the inter-band FS nesting is substantially suppressed in the FM phase. The inter-band scattering between different spins is negligible under the external charge potential of FM ordering. Therefore, FS nesting vector is split and the overall FS nesting feature should be suppressed as each FS has different spin configurations. The detailed analysis will be shown in the calculation of \(\chi_0(q)\).
Figure 5. The change of the FSs under hydrostatic pressure (a), (b) and chemical pressure (c), (d) in the NM phase. Each color classifies different pressure. The plane of the 2D FS plot and the symmetry points are represented in figure 4.

We also investigated the change of the FSs with increasing pressure. The FSs under various pressures are shown in the figure 5 for ab plane (for $q_1$ vector) and diagonal part of ab, ac plane (for $q_R$ vector). Because the chemical and hydrostatic pressures have similar contribution to the FS, a similar effect on the CDW phase is expected. As the pressure increases, the overall FSs become flatter and more 1D like along $a$ direction. This is consistent with the increased conductivity along $a$ direction with the pressure. Despite the flattened FS, the overall FS nesting feature near $\Gamma - X$ line still holds for all the pressure ranges. For this reason, one can predict that the FS nesting feature maintains for all the pressure ranges of our interest. This corresponds to the experimental results where $T_{CDW}$ does not vanish for high pressure over 6 GPa or chemical pressure, such as GdNiC$_2$ and NdNiC$_2$ compounds [3, 8].

3.4. Generalized susceptibility, $\chi_0(q)$

The CDW vector, corresponding to the FS nesting direction, is accurately evaluated by calculating $\chi_0(q)$ using equation (1). Figure 6 shows the plot of $\chi_0(q)$ along (0.5, x, 0) and (0.5, 0.5, x) symmetry lines and the 2D contour plot of $\chi_0(q)$ within (0.5, x, y) plane, where $0 \leq x$, $y \leq 1$. The calculated $\chi_0(q)$ has one significant global maximum peak at $q_1 = (0.5, 0.52, 0)$. This is same as the experimental CDW vector $q_1$ [4] and similar to the previous theoretical work with $q_1 = (0.5, 0.56, 0)$ [9]. Also, there is broad local maximum feature around $q_R = (0.5, 0.5, 0.5)$, which is another weak CDW vector measured in the experiment [4]. However, according to the 2D plot of $\chi_0(q)$ shown in figure 6(b), the $q_R$ vector is a saddle point within a broad plateau containing local maxima points denoted as X near $q_R$. Compared to the prominent peak at $q_1$, the peak at $q_R$ has broad and ambiguous nesting behavior. This result is also consistent with the experimental measurement that x-ray satellite peak along $q_R$ vector is weak, compared with $q_1$ vector [4].

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The suppression of the CDW phase with the FM ordering [4] can be understood with the suppression of the FS nesting with the splitting of the conduction bands. Although previous studies have not shown clear suppression of the FS nesting from the calculated $\chi_0(q)$ [9], figure 6(a) clearly shows the suppressed and broad hump feature (green dotted line) of $\chi_0(q)$ near $q_1$. This result obviously explains that the FS nesting or the CDW phase is destructed by the FM ordering [4]. As already pointed out in the previous section, it is important to consider only the intra-band contribution of $\chi_0(q)$. If we consider both intra- and inter-band contributions, we find similar results to those of the previous studies [9].

Finally, the calculated $\chi_0(q)$s under various pressure in NM phase along (0.5, x, 0), (0.5, 0.5, x) and (0.5, x, 0.5) symmetry lines are summarized in figure 7. Their overall amplitudes are reduced with the pressure because the DOS at the Fermi level decreases as the pressure increases. In figure 7(a), the FS nesting vector $q_1$ is gradually shifted from (0.5, 0.5, 0) at $-6$ GPa to (0.5, 0.55, 0) at 12 GPa as the pressure increases. This shows that $\chi_0(q)$ can capture very small changes of the FSs, as shown in figure 5. Chemical pressure, however, does not affect the direction of the FS nesting vector $q_1 \sim (0.5, 0.52, 0)$. This is quite different from the previous observations where the nesting vector is significantly changed with chemical substitution [9]. The difference between the chemical and the hydrostatic pressure comes from the different changes of FSs near $\Gamma$–$X$ line. Slightly tilted FSs around $\Gamma$ in figure 5(a) changes into clear change of FSs along the $q_1$ direction under hydrostatic pressure, while the change of FSs around $\Gamma$ in figure 5(c) is negligible under chemical pressure.

Figures 7(b), (c) and 8 show $\chi_0(q)$ along different symmetry lines: (0.5, 0.5, x), (0.5, x, 0.5) and (0.5, x, y) for the investigation of the FS nesting around $q_R$. In SmNiC$_2$ at $-6$ GPa and NdNiC$_2$, whose volume corresponds to that of SmNiC$_2$ at $-5$ GPa, there is clear single local maximum peak at (0.5, 0.5, 0.5). However, around the ambient pressure of SmNiC$_2$ this
Figure 7. The calculated $\chi_0(q)$ of SmNiC$_2$ in the NM phase with the change of pressure along (a) $(0.5, x, 0)$, (b) $(0.5, 0.5, x)$, and (c) $(0.5, x, 0.5)$. Each colored line indicates hydrostatic pressure and the black solid lines indicate chemical pressure, which are classified by blue arrows. (a) The black arrow indicates the change of the FS nesting vector $q_1$.

single peak starts to split from the symmetry lines. The amount of splitting becomes larger with increasing pressure. Thus, one can expect that the FS nesting feature along $q_R$ becomes unclear with increasing the pressure, and this leads to the suppression of the CDW phase as increasing pressure.

3.5. CDW strength versus dimensionality

RNiC$_2$ shows different behavior with typical CDW compounds. The $T_{\text{CDW}}$ becomes larger by both chemical and hydrostatic pressure even for high pressure [3, 8]. Some CDW compounds also show increasing $T_{\text{CDW}}$ under pressure [16, 32–34], but it only increases at low pressure. Also, it shows a second CDW phase of decreasing transition temperature ($T_{\text{CDW2}}$) by pressure. In this compound, our band calculation has found that 1D anisotropy along $a$ direction increases under pressure unlike other typical CDW compounds. In addition, the FS nesting along $q_1$ vector
Figure 8. A 2D plot of the $\chi_0(q)$ in $(0.5, x, y)$ plane under hydrostatic (a)–(c) and chemical (d), (e) pressures in the NM phase. The brighter part indicates a higher value of $\chi_0(q)$. The local maximum peaks near $q_1$ and $q_R$ are represented by X.

remains strong, even for high pressure, while the FS nesting along $q_R$ vector becomes ambiguous as pressure increases.

The enhancement of the CDW strength ($T_{CDW}$) along $q_1$ is responsible for the increased 1D anisotropy along $a$ direction. This would hold for high pressure if there is no structural transition. However, the CDW along $q_R$ of second CDW phase shows a complicated feature. Under low pressure, it holds an FS nesting feature with weak nesting along near $(0.5, 0.5, 0.5)$. This corresponds to $T_{CDW2}$. As pressure increases further, it becomes more broadened and $\chi_0(q)$ peak becomes broad plateau, which means suppression of the CDW phase. For chemical pressure cases, there is no experimental analysis for the second CDW phase [3] and more experiments, such as x-ray diffraction experiment [4], are needed.

4. Conclusion

We have investigated the change of the crystal structure, the electronic structures, the FSs, and the $\chi_0(q)$ of SmNiC$_2$ with the existence of magnetism and pressure. At ambient pressure, the NM and FM calculation explains the experimental observation of the construction and destruction of the CDW phase, respectively. In addition, our results are consistent with recent experimental studies under pressure, where multiple CDW transitions are observed [3, 8]. Our electronic structure calculation with pressure suggests that the increased 1D anisotropy along $a$ direction in the electronic structure enhances the CDW strength along $q_1$ and it increases $T_{CDW}$. 

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Also, the additional CDW phase along $q_R$ is suppressed because pressure induces the broadening of the $\chi_0(q)$ peak near the $q_R$ vector.

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