Enhancing the critical temperature of strained Niobium films

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Abstract

The study of the high critical temperature \( T_c \) of hydrogen compounds under high pressure has resulted in a considerable focus on Bardeen–Cooper–Schrieffer superconductors. Nb has the highest \( T_c \) among the elemental metals at ambient pressure, so reviewing Nb films again is worthwhile. In this study, we investigated the factors that determine the \( T_c \) of Nb films by strain introduction and carrier doping. We deposited Nb films of various thicknesses onto Si substrates and evaluated the \( T_c \) variation with thickness. In-plane compressive strain in the (110) plane due to residual stress reduced the \( T_c \). First-principles calculations showed that adjusting the density of states at the Fermi level is key for both strain-induced suppression and doping-induced enhancement of the Nb \( T_c \). The application of hydrostatic pressure compensated for the intrinsic strain of the film and increased its \( T_c \), which could also be enhanced by increasing the hole concentration with an electric double-layer transistor. A liquid electrolyte should be used as a pressure medium for applying hydrostatic pressure to increase the \( T_c \) of correlated materials, where this increase results from changes in material structure and carrier concentration.

1. Introduction

For more than a century, superconductivity has been among the most intensively and extensively studied physical properties driven by the search for materials featuring a critical temperature \( T_c \) near room temperature. Although iron–based and cuprate materials are representative unconventional high-\( T_c \) superconductors, the highest \( T_c \) has been achieved in covalent hydrogen compounds under high pressure [1–5], including Drozdov et al who reported \( T_c \) values of 203 K for \( \text{H}_3\text{S} \) at 155 GPa and approximately 250 K for \( \text{LaH}_{10} \) at 150 GPa [6, 7]. Hydrogen superconductors exhibit the isotope effect, which is typical for conventional phonon-mediated (i.e., Bardeen–Cooper–Schrieffer; BCS) superconductors [8]. This result agrees well with the BCS theory that suggests metal–hydrogen and hydrogen compounds are promising candidates for high-\( T_c \) superconductors due to high phonon frequencies [9–13]. The recent discovery of high \( T_c \) in hydrogen compounds has led to renewed interest in BCS superconductors as well as research into increasing \( T_c \) [14–19].

In the standard BCS theory, \( T_c \) is estimated as

\[
T_c = 1.14 \Theta_D \exp \left( -\frac{1}{N(0)V} \right),
\]

where \( \Theta_D \) is the Debye temperature, \( N(0) \) is the density of states (DOS) at the Fermi level \( (E_F) \), and \( V \) is the electron–phonon coupling potential. The high \( T_c \) of covalent compounds originates from a high \( \Theta_D \), which in turn is due to a light ionic mass [20]. Equation (1) indicates that the \( T_c \) of materials can be controlled by changing the DOS at \( E_F \) via chemical substitution and modification of lattice dynamics. The control of the lattice constants of materials through, for example, the application of hydrostatic and uniaxial pressure to bulk or epitaxial film growth on the substrate can alter the electronic band and phonon properties of the materials [21, 22].

Several studies have examined \( T_c \) tuning by varying the thickness of Nb thin films. Nb is a BCS superconductor with a body-centered cubic (bcc) structure, and bulk Nb has the highest \( T_c \) (≈9.25 K) among
 elemental superconductors at ambient pressure \([23]\). \(T_c\) suppression in thick Nb films deposited on Si substrates has been attributed to the size reduction of the superconducting crystalline grains, specifically, the proximity of the quantum size effect \([24–26]\). Because high-quality epitaxial Nb thin films deposited on sapphire or MgO substrates exhibit a \(T_c\) as high as that of bulk Nb, \(T_c\) suppression occurs only in the region of reduced length scale, or where the film thickness is lower than the Nb coherence length \((\xi_{\text{Nb}} = 38 \text{ nm})\) \([27–30]\). \(T_c\) tuning can also be achieved through charge carrier doping, which changes the DOS at \(E_F\) \([31–33]\). Furthermore, the improvement of the Nb film \(T_c\) by an electric double-layer transistor (EDLT) has been actively studied. Choi et al. successfully controlled the \(T_c\) of Nb thin films deposited on sapphire substrates with the EDLT method \([27]\) and achieved a tunable \(T_c\) range of approximately 80 mK while also modulating the superconducting critical current. Tsuchiya et al. developed a new approach, called the all-solid-state EDLT, based on the use of Li4SiO4 and LiCoO2 as the solid electrolyte and gate electrode, respectively \([34]\). However, these studies both raised questions about the cause of \(T_c\) suppression in the bulk Nb system, which cannot be elucidated by the simple electrostatic effect or the cause of \(T_c\) enhancement via the EDLT method for thick Nb films. Despite these unsolved issues, the findings from these previous efforts helped improve our understanding of BCS superconductors.

In this study, we investigate the factors determining the \(T_c\) of Nb films on Si substrates. The \(T_c\) was suppressed when the deposition time was shortened as the Nb film thickness was reduced. However, this thickness is not within a reduced length scale, so the \(T_c\) of the Nb film should be constant and the same as that of bulk Nb. To discover the reason for this \(T_c\) suppression, we studied the effect of the in-plane compressive strain via x-ray diffractometry (XRD) and temperature-dependent resistivity \((\rho(T))\) measurements. In addition, first-principles calculations demonstrate that strain-induced structural transformations could modify the DOS at the Fermi level, resulting in a change in \(T_c\), while carrier doping could modify the DOS without structural deformation. These calculations also predict that hole doping would increase the \(T_c\). Based on these results, we performed two experiments to examine if \(T_c\) could be enhanced by (1) compensating for the intrinsic \(T_c\) reduction resulting from hydrostatic-pressure-induced deformation and (2) through carrier doping via electric double-layer (EDL) gating.

2. Experimental details

Nb films were grown on Si substrates via direct current magnetron sputtering. A P-type Si (100) wafer was cut into 10 \(\times\) 10 mm\(^2\) squares and rinsed by acetone, ethanol, and distilled water for 15 min each. The wafer was 530 \(\mu\)m thick and retained its native oxide layer. The base vacuum level was fixed at 1.0 \(\times\) 10\(^{-5}\) Torr and the film was grown at an argon pressure of 1.6 mTorr with an Ar gas flow rate of 20 sccm. At an optimal substrate temperature (240 \(^\circ\)C) and power (210 W) previously reported, Nb films of various thicknesses were deposited by adjusting the sputtering time \([35]\). The film thickness was measured by a field-emission scanning electron microscopy system (Hitachi SU8220). XRD 2\(\theta\)/\(\omega\) scans were performed in the 30\(^\circ\)–90\(^\circ\) range with a PANalytical XPert Pro diffractometer. \(\rho(T)\) was measured by heating the Nb films at a rate of 0.1 K min\(^{-1}\) up to a temperature close to the \(T_c\) with a resistance bridge measured using a four-point probe method positioned at the middle of the Nb film. The temperature of the sample in vacuum was controlled by cooling through a 4 K cryocooler (Sumitomo RDK-101D) and heating block connected to a Lakeshore 336 temperature controller. The \(T_c\) was derived from the maximum value of the first derivative of \(\rho(T)\). \(N,N\)-diethyl-\(N\)-methyl-\(N\)-(2-methoxyethyl)ammonium bis(trifluoromethylsulfonyl)imide ([DEME][TFSI]) was used as the ionic liquid for EDL gating. To prevent chemical reactions, a gate voltage was applied at 240 K and increased gradually by 0.005 V s\(^{-1}\). In addition, the leakage current between the Nb film and the gate electrode was monitored simultaneously. The pressure experiment was performed in a piston-cylinder cell with [DEME][TFSI] as the pressure medium instead of Daphne oil 7373, which is typically used because of its good tolerance to solidification under high pressure, as [DEME][TFSI] has a viscosity similar to that of Daphne oil 7373. The gate voltage was applied under pressure. Pure Pb and manganin wires were used as a pressure manometer.

The electronic structure and electron–phonon coupling (EPC) calculations were performed by the Quantum ESPRESSO software \([36]\) with the pseudopotential band method and density functional perturbation theory \([37]\). The projected augmented wave Perdew–Burke–Ernzerhof functional was selected as an exchange-correlation functional \([38, 39]\). The kinetic energy cutoff for the wave functions was 50 Ry. For the EPC calculations, we used a 6 \(\times\) 6 \(\times\) 6 q-mesh and 36 \(\times\) 36 \(\times\) 36 high-density k-mesh, then optimized the lattice parameters and atomic positions of the initial bcc structure \([40]\) with a fixed volume to consider strained structures. We modeled the experimental in-plane compressive strain in the (110) plane with a simple body-centered tetragonal (bct) structure. With this compressive strain in the (110) plane, the lattice constant decreases, and the \(a (=b)\) lattice constant increases while maintaining the volume similar to the original cell. The strained bct structures were generated with the same volume as the unstrained bcc structure. The in-plane
compressive and tensile strains corresponded to the bct structures compressed and stretched, respectively, along the c direction.

3. Results and discussion

Figure 1 (a) shows the XRD patterns of various samples with the (110) and (220) diffraction peaks of bcc Nb films and the Si(004) diffraction peak. The Nb peaks of the films were well-matched, while the Nb signal varied with film thickness. In particular, the Nb(110) peak shifted toward a lower 2θ when the film thickness decreased, as shown in figure 1 (b). The 2θ value of bulk cubic Nb(110) is 38.214° (JPCDS card no. 96–411–1970), and a lower 2θ indicates an extended d-spacing of Nb(110) corresponding to the in-plane compressive strain in the (110) plane. Figure 1 (c) shows resistivity measurements of the Nb films near the $T_c$, $\rho(T)$, suggesting that the thinner the film, the higher is the resistivity and the greater the $T_c$ suppression. Figure 1 (d) shows the correlation between the 2θ of the Nb(110) peak, the film thickness, and the $T_c$ for all samples. However, we found that the samples represented by the open square did not exhibit a superconducting transition regardless of thickness. Two samples have a 2θ lower than 37.2 degrees but a thickness two or three times larger than the coherence length of Nb. In addition, the highest $T_c$ was achieved in the second thickest sample, suggesting that $T_c$ is not directly
related to the film thickness. Notably, the $T_c$ value demonstrated greater correlation with the shift of $2\theta$ caused by the compressive strain compared to its correlation with the film thickness.

The stress and strain in films deposited through physical vapor deposition tend to be influenced by various reasons, including mismatches in the thermal expansion coefficients, large lattice mismatches \([41, 42]\), and Ar-ion bombardment. As a result, intrinsic strain occurs uniformly in films and influences the curvature of both the substrate and films. Moreover, the films had residual stress because of uniform compressive or tensile strain. Because we used a Si substrate with its native oxide layer, and all depositions were performed with the same substrate temperature, the energetic ion bombardment during deposition was expected to be a primary reason for intrinsic strain. The structural deformation from the ion bombardment was effective on thinner films, which resulted in compressive residual stress and a convex-up curvature.

To investigate the effect of uniform strain on the superconducting properties of Nb, we performed density functional theory (DFT) calculations. $T_c$ was computed using the Allen–Dynes formula \([43]\),

$$T_c = \frac{\omega_{\log}}{1.20} \exp \left[ \frac{-1.04 (1 + \lambda)}{(\lambda (1 - 0.62 \mu^*) - \mu^*)} \right] \quad (2)$$

where $\mu^*$ is the effective Coulomb repulsion parameter, $\lambda$ is the EPC constant, and

$$\omega_{\log} = \exp \left[ \frac{1}{2} \int \frac{d\omega}{\omega} \alpha^2 F(\omega) \log \omega \right]$$

with $\alpha^2 F(\omega)$ being the Eliashberg function. The as-calculated $T_c$ of the bcc Nb for $\mu^* = 0.21$ was 9.95 K (see table 1), which is consistent with the experimental value of 9.25 K reported above. We used a $\mu^*$ value larger than the typical values of 0.1 or 0.13 to reproduce the experimental $T_c$ of Nb. Nb required a large $\mu^*$ as in previous theoretical studies ($\mu^* = 0.22$ in \([44]\) and 0.21 in \([45]\)), and the tunneling data also reported $\mu^*$ in a range of 0.15–0.19 \([46]\). Therefore, we believe that a $\mu^*$ of 0.21 for Nb can be valid despite being greater than the typical empirical value of 0.1 or 0.13.

Figure 2 shows the DOS at $E_F$ ($N(E_F)$) and the corresponding $T_c$ as functions of the strain (%), calculated as

\[ N(E_F) \times 100\% \]

The experimental in-plane compressive and tensile strains in the (110) plane correspond to the positive and negative values, respectively. $N(E_F)$ and $T_c$ exhibited the same decreasing trend with increasing compressive and tensile strains, implying that the strain-induced transformation from a cubic to a tetragonal structure reduced the number of electrons participating in the pairing mechanism, resulting in a decrease in the $T_c$.

According to the BCS theory, $T_c$ can be enhanced by increasing $N(E_F)$. Therefore, we performed DFT calculations with different doping concentrations, and we removed or added electrons by inserting a compensating charge background to maintain the charge neutrality of the system. Figure 3(a) shows the calculated $N(E_F)$ results for bcc Nb without any carrier doping, which are consistent with those previously measured via angle-resolved photoemission spectroscopy for an Nb thin film \([47]\). A peak in the DOS near $E_F$
occurred below $E_F$. Therefore, hole doping up to 0.4 holes/Nb atom lowered the Fermi level and increased $N(E_F)$, reinforcing the electron–phonon interactions. Figure 3(b) shows the corresponding $N(E_F)$ and EPC constant as functions of the carrier doping. Both reached maximum values at 0.4 holes/Nb atom. Moreover, the $T_c$ increased up to 15.1 K (figure 3(c)). On the other hand, in the case of electron doping, $N(E_F)$ decreased, reducing the $T_c$.

Our DFT calculations suggest two experimental approaches to increase the $T_c$, including compensating for the $T_c$ reduction due to pressure-induced film deformation and increasing $N(E_F)$ by adjusting the Fermi level. One of the most effective ways to change $E_F$ is via ionic liquid gating that facilitates a carrier concentration ten times higher than that achieved with conventional (dielectric) field-effect transistors, without structural deformation. The process, called electrostatic doping, is reversible, and, therefore, both electron and hole doping can be performed on the same sample. When a gate voltage is applied to the ionic liquid between the anode and the gate electrode, the cations or anions are driven by the electric potential toward the sample surface.

Depending on the gate voltage polarity, the electron or hole concentration at the ionic liquid surface is largely modulated. Ionic liquid gating was performed in the order of 0 V, −5 V, 0 V, 3 V, and 0 V. Figure 4(a) shows temperature-dependent resistance ($R(T)$) near the $T_c$ for each voltage. Initially (i.e., without a gate voltage being applied), the $T_c$ reached approximately 9 K (black curve). After the film reached room temperature at which the ionic liquid was liquefied, a negative bias voltage of −5 V was gradually applied at 230 K. The [DEME][TFSI] exhibited a rubbery transition at 240 K and a glass transition at 182 K [49] where the ionic motion slowed down during the rubbery phase and disappeared at the glassy phase. $R(T)$ at −5 V revealed an enhanced $T_c$, while the $T_c$ at 3 V was reduced, following the DOS calculation results. To confirm the doping reversibility, the same procedure was conducted after removing the bias voltage. Hole doping was reversible, with $T_c$ returning to the initial value (red curve), whereas electron doping was not (blue curve). This observed irreversibility can be attributed to an unexpected chemical reaction between the ionic liquid and the Nb thin film, which acted as the anode. During the application of a positive bias voltage, the leakage current monitored suddenly increased to over several hundred nA (inset of figure 4(a)), and the bias voltage was adjusted to a maximum of 3 V.

The $T_c$ of Nb films can be enhanced by reducing the film deformation. Because $T_c$ suppression is related to film bending, we applied a hydrostatic pressure to restore the deformation of the convex-up film. Previous reports showed that the $T_c$ of the Nb films increased under hydrostatic pressure, whereas that of bulk Nb decreased [50, 51]. A monotonic decrease in $T_c$ up to about 5 GPa, where the Lifshitz transition occurs for bulk Nb, could be related to structural deformation [52]. In addition, EDL gating could be performed under pressure.
using an ionic liquid as a pressure medium. Pressurizing the ionic liquid increased the glass transition temperature where, according to the pressure-temperature phase diagram of [DEME][TFSI], its glass transition temperature reaches 260 K at 0.6 GPa [53]. Thus, about 1 GPa, we applied a gate voltage at 310 K and increased it gradually by 0.005 V s⁻¹, while monitoring the leakage current. The results of the hydrostatic pressure and doping on two Nb films with different $T_c$ values of 8.37 K and 9.13 K are shown in figures 4 (b) and (c), respectively. The sample in figure 4 (b) was the same as the one in figure 1 (d) with a thickness of 709.8 nm and having the highest $T_c$. However, extrinsic strain was induced by cutting the film to the size inside the pressure cell, leading to superconducting transition broadening and $T_c$ degradation. Consequently, we fabricated a second sample after cutting the Si substrate into small pieces to avoid extrinsic strain. The SC transition became sharper with higher $T_c$ ($\approx$ 9.13 K) at ambient pressure and 0 V, as shown in figure 4 (c). Figure 4 (b) shows the pressure and voltage dependence of the $T_c$ in a low-$T_c$ film. The $T_c$ increased with hole doping (ambient pressure, $-1$ V) and pressurization (1.3 GPa, 0 V). However, at 1.3 GPa, the value at $-5$ V was nearly identical to that at 0 V, indicating the absence of the ionic doping effect. The $T_c$ at 1.27 GPa and $-10$ V increased slightly. Nonetheless, this increase might not have originated from the electrostatic doping because the intercalation of ions (e.g., sulfur and nitrogen) could have occurred at large bias voltages ($\geq$ 5 V). In figure 4 (c), hole doping resulted in a slight increase in $T_c$ only around the onset of $T_c$ (ambient pressure, $-1$ V). At 1.0 GPa, the superconducting transition was significantly broadened. Thus, the $T_c$ onset varied considerably, whereas little difference was observed in its offset (1.0 GPa, 0 V). In contrast to the pressure effect, the effect of hole doping at 1.0 GPa was observed around the offset instead of the onset (1.0 GPa, $-4$ V). Although the $T_c$ was only slightly enhanced, the gating effect could be observed at 1.0 GPa. Though we did not observe a dramatic $T_c$ increasing effect, such as a higher $T_c$ compared to that of bulk Nb, increasing $N(E_F)$ via simultaneous hydrostatic pressure and hole doping was confirmed to provide a $T_c$ enhancement.

4. Conclusions

We experimentally and theoretically studied the enhancement of the $T_c$ of Nb films via strain introduction and carrier doping. We controlled the film thickness by adjusting the deposition time and observed a decrease in the $T_c$ of thinner samples. The spacing between the Nb(110) planes increased as the film thickness decreased, revealing an in-plane compressive strain in the (110) plane of the film. The DFT calculations suggested that
decreasing $N(E_F)$ by introducing strain suppressed $T_c$. Furthermore, we examined the effect of the carrier concentration on the $T_c$, and calculations predicted a $T_c$ enhancement with increases in $N(E_F)$. Based on calculations, two superconductivity-tuning methods were investigated for the fabricated Nb thin films, including (1) compensating the suppressed superconductivity by applying hydrostatic pressure to release the film bending and (2) enhancing the superconductivity by generating a field-induced hole-doping effect with an ionic liquid. We attempted to combine these two methods by using an ionic liquid as a pressure medium. However, the efficacy of this combination could not be fully confirmed because the ionic liquid could not maintain an electrostatic state at high pressure. Nonetheless, we demonstrated that the superconductivity of Nb thin films deposited on Si substrates could be controlled through the fabrication conditions and by increasing $N(E_F)$ via hydrostatic pressure application and hole doping. This method, which changes both the film structure and doping level simultaneously, could be helpful for future investigations of high-$T_c$ correlated materials.

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**References**

[1] Keimer B, Kivelson S A, Norman M R, Uchida S and Zaanen J 2015 Nature 518 179
[2] Yanagisawa T 2019 Condensed Matter 457
[3] Camargo-Martínez J A, González-Pedero G I and Baquero R 2019 Supercond. Sci. Technol. 32 125013
[4] Einaga M, Sakata M, Ishikawa T, Shimizu K, Eremets M I, Drozdov A P, Troyan I A, Hirao N and Ohishi Y 2016 Nat. Phys. 12 835
[5] Erema et al 2015 Phys. Rev. Lett. 114 157004
[6] Drozdov A P, Eremets M I, Troyan I A, Ksenofontov V and Shylin S I 2015 Nature 525 73
[7] Drozdov A P et al 2019 Nature 569 528
[8] Gor’Kov L P and Kresin V Z 2018 Rev. Mod. Phys. 90 011001
[9] Eremets M I, Troyan I A, Medvedev S A, Tse J S and Yao Y 2008 Science 319 1566
[10] Cudazzo P, Profeta G, Sanna A, Floris A, Continenzia A, Massidda S and Gross E K U 2008 Phys. Rev. Lett. 100 257001
[11] Peng F, Sun Y, Pickard C J, Needs R J, Wu Q and Ma Y 2017 Phys. Rev. Lett. 119 107001
[12] Salke N P et al 2019 Nat. Commun. 10 4453
[13] Martínez-Canales M, Oganov A R, Ma Y, Yan Y, Lyakhov A O and Bergara A 2009 Phys. Rev. Lett. 102 087005
[14] Ashcroft N W 1968 Phys. Rev. Lett. 21 1748
[15] Ashcroft N W 2004 Phys. Rev. Lett. 92 187002
[16] Ghosh S S, Quan Y and Pickett W E 2019 Phys. Rev. B 100 094521
[17] Li Y, Hao J, Liu H, Tse J S, Wang Y and Ma Y 2015 Sci. Rep. 5 9948
[18] Duan D et al 2015 Sci. Rep. 4 6968
[19] Tse J S, Yao Y and Tanaka K 2007 Phys. Rev. Lett. 98 117004
[20] Naito M and Ueda K 2004 Supercond. Sci. Technol. 17 R1
[21] Zheng J C and Zhu Y 2006 Phys. Rev. B 73 024509
[22] Huang M Z, Xu Y N and Ching W Y 1993 Phys. Rev. B: Condens. Matter 47 8249
[23] Finnemore D K, Stromberg T F and Swenson C A 1966 Phys. Rev. 149 231
[24] Bose S, Banerjee R, Genc A, Raychaudhuri P, Fraser H L and Ayyub P 2006 J. Phys. Condens. Matter 18 4553
[25] Bose S, Raychaudhuri P, Banerjee R, Vasa P and Ayyub P 2005 Phys. Rev. Lett. 95 147003
[26] Gubin A I, Jin K S, Virtusewich S A, Siegel M and Klein R 2005 Phys. Rev. B 72 064503
[27] Choi J, Pradhanesh H K, Kim H, Im H, Chong Y and Chae D H 2014 Appl. Phys. Lett. 105 012601
[28] Roach W M, Beringer D B, Skuza J R, Oliver W A, Clavero C, Reece C E and Lukasiew R A 2012 Physical Review Special Topics—Accelerators and Beams 15 062002
[29] Delacour C, Ortega L, Faucher M, Crozes T, Fourrier T, Pannetier B and Bouchiat V 2011 Phys. Rev. B 83 144504
[30] Clavero C, Beringer D B, Roach W M, Skuza J R, Wong K C, Batchelor A D, Reece C E and Lukasiew R A 2012 Crystal Growth & Design 12 2588
[31] Glover R E and Sherrill M D 1960 Phys. Rev. Lett. 5 248
[32] Bollinger A T, Dubuis G, Yoon J, Pavuna D and Bozovic J 2011 Nature 472 458
[33] Dubuis G, Bollinger A T, Pavuna D and Bozovic J 2011 Appl. Phys. Lett. 111 112632
[34] Tsuchiya T, Moriyama S, Terabe K and Aono M 2015 Appl. Phys. Lett. 107 013104
[35] Choi J, Lee J, Kim C D, Jo Y, Kang J, Ba S H, Yang J and Jeong D 2018 New Physics: Sae Mulli 68 284
[36] Giannozzi P et al 2009 J. Phys. Condens. Matter 21 395502
[37] Baroni S, De Gironcoli S, Dal Corso A and Giannozzi P 2001 Rev. Mod. Phys. 73 515
[38]Blochl P E 1994 Phys. Rev. B 50 17953
[39] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[40]Schimml H G, Huot J, Chapon L C, Tichelaar F D and Mulder F M 2003 JACS 127 14348
[41]Windischmann H 1992 Crit. Rev. Solid State Mater. Sci. 17 347
[42]Motazedian F, Wu Z, Zhang J, Samsam Shariat B, Jiang D, Martyniuk M, Liu Y and Yang H 2019 Mater. Des. 181 108063
[43]Allen P B and Dynes R C 1975 Phys. Rev. B 12 905
[44]Peña-Seaman O D L, De Coss R, Heid R and Bohnen K P 2007 J. Phys. Condens. Matter 19 476216
[45]Savrasov S Y and Savrasov D Y 1996 Phys. Rev. B 54 16487
[46]Geerk J, Gurvitch M, McWhan D B and Rowell J M 1982 Physica B + C 109–110 1775
[47]Xiang P, Liu J-S, Li M-Y, Yang H-F, Liu Z-T, Fan C-C, Shen D-W, Wang Z and Liu Z 2017 Chin. Phys. Lett. 34 077402
[48]Ueno K, Shimotani H, Yuan H, Ye J, Kawasaki M and Iwasa Y 2014 J. Phys. Soc. Jpn. 83 032001
[49]Fujimoto T and Awaga K 2013 Phys. Chem. Chem. Phys. 15 8985
[50]Pristaš G, Gabáni S, Gažo E, Komanický V, Orendač M and You H 2014 Thin Solid Films 556 470
[51]Smith T F 1970 Phys. Lett. A 33 465
[52]Struzhkin V, Timofeyev Y, Hemley R and Mao H-K 1997 Phys. Rev. Lett. 79 4262
[53]McCann D M, Misiek M, Kamenev K V and Huxley A D 2015 Phys. Proc. 75 252