Superconducting properties of the ternary transition-metal silicide Zr$_2$Ru$_3$Si$_4$

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Abstract
Superconducting properties of the polycrystalline Zr$_2$Ru$_3$Si$_4$ were investigated by measuring the electrical resistivity, magnetization and specific heat. By these measurements, bulk superconductivity with transition temperature $T_c = 5.5$ K was confirmed. Moreover, Zr$_2$Ru$_3$Si$_4$ was found to be a type-II and intermediate-coupling superconductor. Interestingly, the electronic specific heat shows a deviation from a one-gap s-wave model and $H_{c2}(T)$ shows unusual positive curvature in the vicinity of $T_c$. The electronic structure calculation shows the existence of plural anisotropic Fermi surfaces. These results suggest that Zr$_2$Ru$_3$Si$_4$ is not an isotropic single-gap superconductor, but possibly a multi-gap or an anisotropic gap superconductor.

Keywords: multi-gap superconductivity, anisotropic gap superconductivity, electrical resistivity, magnetization, specific heat

1. Introduction
Superconductivity in the ternary silicides R$_x$T$_y$Si$_z$ containing a rare-earth element R and a transition element T was explored with an expectation of finding new examples of interactions between superconductivity and magnetism at the end of the 1970s and in the 1980s [1]. In this period, superconductors with various attractive features were discovered, such as the first heavy fermion superconductor (CeCu$_2$Si$_2$ [2]), multi-gap superconductors (Lu$_2$Fe$_2$Si$_5$ [3, 4] and Sc$_3$Ir$_4$Si$_{10}$ [5, 4]) and a noncentrosymmetric superconductor (LaPtSi [6, 1, 7, 8]). Reflecting these successful results, the efforts searching for new superconductors in R$_x$T$_y$Si$_z$ have continued until now.

The ternary Zr–Ru–Si system has not yet been fully investigated and has been reported only in two compounds: ZrRuSi [9] and Zr$_2$Ru$_3$Si$_4$ [10]. Their physical properties are little known. An ambient phase of ZrRuSi synthesized by arc melting has been reported to show no superconductivity down to 1.2 K [11, 12], while that synthesized at a high pressure shows it with $T_c$ of 7–12 K [13], although it is isostructural to the ambient phase. Additionally, another high-pressure phase of ZrRuSi has been reported to be a superconductor with $T_c$ of 3–5 K [13]. As for Zr$_2$Ru$_3$Si$_4$, superconductivity with $T_c$ of 5.6 K was originally reported in a half page abstract for a presentation by Braun et al in 1986 [14, 15], but no detail has been reported so far. Zr$_2$Ru$_3$Si$_4$ has the Hf$_2$Ru$_3$Si$_4$-type structure (space group $C2/c$, monoclinic) with $a = 19.0$, $b = 5.34$, $c = 13.3$ Å and $\beta = 127.73^\circ$ [10]. The structure is characterized by infinite columns of face-shared Ru-centred Si-octahedra and infinite columns of face-shared Si-centred square antiprisms [16]. Three compounds, Hf$_2$Ru$_3$Si$_4$ [10], Yb$_2$Ru$_3$Ge$_4$ [17] and Zr$_2$Ru$_3$Si$_4$ [10], are known to crystallize in this structure; only Zr$_2$Ru$_3$Si$_4$ was reported to be a superconductor above 1.8 K among the three compounds.

Thus, in this study, we investigated the superconducting properties of the polycrystalline Zr$_2$Ru$_3$Si$_4$ by electrical resistivity, magnetization and specific heat measurements. From these measurements, we established bulk superconductivity with $T_c = 5.5$ K. The field dependence of the magnetization characterizes it as type-II superconductivity. Additionally, specific heat and $H_{c2}(T)$ results suggest that Zr$_2$Ru$_3$Si$_4$ is not a simple s-wave superconductor, but is probably a multi-gap or an anisotropic gap superconductor, attributed to the low-symmetric structure.

2. Material and methods
Polycrystalline Zr$_2$Ru$_3$Si$_4$ was prepared by arc melting and subsequent annealing. The starting materials of 99.9% purity for Zr, 99.9% for Ru and 99.99999999% for Si were...
weighted with the molar ratio of Zr:Ru:Si = 20:35:45 and melted on a water-cooled copper hearth under high purity argon gas atmosphere. The proportion of Ru and Si to Zr was increased from the stoichiometric composition 2:3:4 to decrease ZrRuSi impurity. The resulting as-cast alloy was put in an alumina crucible, sealed in a quartz tube under a pure Argon atmosphere, and heat-treated at 1273 K for 100 h in an electric furnace. The sample was cooled down in the furnace by turning off the heater. The annealed sample was characterized by x-ray powder diffraction (RINT TTR-III, Rigaku) with Cu Kα radiation and electron probe microanalyzer (JXA-8500F, JEOL). Atomic compositions were determined by wave dispersive x-ray spectroscopy. The sample was cut into rectangles for each measurement. A four-probe electrical resistivity measurement was employed by using the PPMS. The sample was mounted on a specially designed plug and inserted into a Teflon cell with Daphne 7373 (Idemitsu Kosan Co.) pressure-transmitting media. Generated pressure in the cell was calibrated against the load using Tc of Pb [19]. The temperature at the sample position was measured using an extra calibrated thin film resistance sensor (Cernox, Lake Shore Cryotronics). Two sets of the measurements were performed from low to high pressures using the same sample. Additionally, band structure, electronic density of states (DOS) and Fermi surfaces of Zr2Ru3Si4 were calculated by the DFT-based plane-wave basis sets and ultrasoft pseudopotentials method [20] implemented in the Quantum-ESPRESSO package [21]. The plane-wave energy cutoff was set to 25 Ryd. The structural parameters of Zr2Ru3Si4 were fixed at the experimentally observed values in [10]. Zr (4s, 4p, 4d, 5s, 5d), Ru (4d, 5s, 5p) and Si (3s, 3p) were treated as valence electrons. For the exchange–correlation functional, the Perdew–Burke–Ernzerhof semi-local density generalized-gradient approximation [22] was used. The Brillouin zone was sampled with Monkhorst–Pack 20×10×20 k-point grids [23]. The total energy convergence was confirmed to be within 3 meV/atom.

3. Results

Figure 1(a) shows the x-ray diffraction pattern of the prepared sample Zr2Ru3Si4, compared with a calculated pattern of the structure reported by Chabot et al [10]. Except for a few peaks, all the peaks were identified as Zr2Ru3Si4. Lattice parameters are a = 18.98, b = 5.348, c = 13.28 Å and β = 127.73°, which are consistent with those reported [10].

The other peaks were identified as ZrRuSi and RuSi, which indicate the existence of the contaminating phases. Figure 1(b) shows a back-scattered electron composition image of Zr2Ru3Si4. Composition of the largest grey area is Zr:Ru:Si = 21.8(3):32.9(4):45.3(2), which is consistent with the stoichiometric composition of Zr2Ru3Si4 within errors. The white phase surrounded by Zr2Ru3Si4 is ZrRuSi. The two dark areas are eutectic phases of Zr2Ru3Si4 and RuSi, and of RuSi and Ru2Si3. We note that neither RuSi nor Ru2Si3 is a superconductor [24, 25]. Additionally, we verified that ZrRuSi, prepared by arc melting, does not show superconductivity down to 1.8 K as described in [11, 12]. These impurities occupy about 10 vol% of the sample. These results indicate that Zr2Ru3Si4 was formed as the major phase in the prepared sample.

Figure 2(a) shows the temperature dependence of the electrical resistivity ρ of Zr2Ru3Si4 from T = 10 to 1.8 K. This displays the steep decrease at 6.0 K and zero resistivity at 5.5 K, indicating the superconducting transition. The inset shows the high-temperature data. The resistivity at 300 K is 240 × 10−6 Ω cm and decreases with temperature going down, indicating the metallic nature of the sample. The residual resistivity ratio ρ(300 K)/ρ(6.1 K) is 4.7. The
Temperature dependence of the resistivity shows negative curvature ($d^2\rho/dT^2 < 0$), and is very different from the Bloch–Grüneisen theory. Such observations were made in many superconductors such as in Nb$_3$Sn and may be attributed to a strong electron–phonon interaction [26–28]. Temperature dependence of the dc magnetic susceptibility $\chi$ with an applied field $H$ being 10 Oe is shown in figure 2(b). $\chi$ decreases at 5.7 K and shows the large diamagnetism both in the zero field cooling (ZFC) and field cooling (FC) processes, indicating the superconducting transition of Zr$_2$Ru$_3$Si$_4$, not of impurities. The shielding volume fraction is about 100% and flux exclusion volume is 10%. The inset shows mass magnetic susceptibility $\chi_M$ in high temperatures with $H = 1000$ Oe. $\chi_M$ is $2.08 \times 10^{-6}$ emu g$^{-1}$ Oe$^{-1}$ at 300 K and shows almost no temperature dependence, indicating the Pauli paramagnetic character. The small up-turn at low temperatures would be attributed to the magnetic impurities. Specific heat $C$ under the applied magnetic field $H$ up to 50 kOe is shown in figure 2(c). A clear jump was found below 5.8 K with $H = 0$ kOe, and it was compressed to lower temperatures by increasing $H$. The result confirmed a bulk superconductivity with $T_c = 5.5$ K in Zr$_2$Ru$_3$Si$_4$. Here, we note that the other two intermetallic compounds with the Hf$_2$Ru$_3$Si$_4$-type structure, Hf$_2$Ru$_3$Si$_4$ and Yb$_2$Ru$_3$Ge$_4$, prepared by arc melting, did not show superconductivity down to 1.8 K in our magnetic susceptibility measurements (not shown). To determine the electron and phonon contributions, the temperature dependence of normal state $C$ at $H = 0$ kOe was fitted to the function $C_{\text{normal}} = \gamma T + \beta T^3 + \delta T^5$, where $\gamma T$ is the electronic term, and $C_{\text{ph}} = \beta T^3 + \delta T^5$ represents the phonon term. The best fitting between 6 K $< T < 10$ K is shown by the solid line in figure 2(c), which yields $\gamma = 13.1$ mJ mol$^{-1}$ K$^{-2}$, $\beta = 0.279$ mJ mol$^{-1}$ K$^{-4}$ and $\delta = 0.0011$ mJ mol$^{-1}$ K$^{-6}$. From $\beta$, the Debye temperature $\theta_D$ was estimated to be 191 K by the relation $\theta_D = [(12\pi^4/5)(Nk_B/\beta)]^{1/3}$, where $N$ is the number of atoms, and $k_B$ is the Boltzmann constant. The existence of the $\delta$ suggests a complex phonon density of states. To analyse the electronic specific heat, the phonon contribution $C_{\text{ph}}$ was subtracted from $C$ with $H = 0$ kOe, and temperature dependence of $(C - C_{\text{ph}})/T$ was examined by the three models: the one-gap $\alpha$-model, the exponential function model and the two-gap $\alpha$-model. $(C - C_{\text{ph}})/T$ is shown in figure 2(d). Firstly, $(C - C_{\text{ph}})/T$ in the superconducting state was fitted to the one-gap $\alpha$-model [29] with the exponential function $C_{\text{one}}(T) \propto \exp(\Delta(0)/(k_B T))$, where $\Delta(0)$ stands for the superconducting gap size at $T = 0$ K. The dotted line in the figure shows the fitting result. The left inset shows $C - C_{\text{ph}}$ as a function of $T_c/T$ with semi-logarithmic scale. The right inset shows the differences between the observed data $(C - C_{\text{ph}})/T$ and fits.

Figure 2. (a) Temperature dependence of the electrical resistivity $\rho$ of Zr$_2$Ru$_3$Si$_4$ at low temperatures. The inset shows $\rho$ up to $T = 300$ K. (b) Temperature dependence of the dc magnetic susceptibility $4\pi \chi$ measured with $H = 10$ Oe. FC and ZFC stand for field cooling and zero field cooling, respectively. The inset shows the temperature dependence of the mass magnetic susceptibility $\chi_M$ measured with $H = 1000$ Oe up to $T = 300$ K. (c) Temperature dependence of the specific heat $C$ under the applied magnetic field $H = 0, 10, 20, 30$ and 50 kOe. The solid line shows the best fit to $C(0 \text{kOe}) = C_{\text{normal}} = \gamma T + \beta T^3 + \delta T^5$. (d) Phonon-subtracted specific heat $(C - C_{\text{ph}})/T$ at $H = 0$ K. The dotted, solid and dashed–dotted lines show the one-gap, two-gap and power law fit, respectively. The left inset shows the inverse temperature dependence of $C - C_{\text{ph}}$. The dotted line shows the one-gap fit. The right inset shows the differences between $(C - C_{\text{ph}})/T$ and fits.
fit the data to the phenomenological two-gap α-model [30]. In this model, the total electronic specific heat is given by the sum of the contributions of each band, \( C_{\text{ELEC}}(T) \propto xC_1(T) + (1 - x)C_2(T) \), where \( C_1(T) = \exp \left( \alpha / (k_B T) \right) \) and \( C_2(T) = \exp \left( \beta T / (k_B T) \right) \); they are electronic specific heat from band 1 and 2, respectively. \( x \) and \( (1 - x) \) are the relative weights for bands 1 and 2, respectively. Interband transitions due to scattering by impurities or phonons are neglected. This model has been successfully applied to MgB\(_2\) [30], borocarbide superconductors [31], Lu\(_2\)FeSi\(_4\) [4], etc. The best fit in the two-gap model is shown by the solid line in figure 2(d), yielding \( \Delta_1 / k_B = 13.7 \) K, \( \Delta_2 / k_B = 5.5 \) K and \( x = 0.9 \). The two-gap fit gives better agreement with the observed specific heat than that of the one-gap model, although this fit has some uncertainty due to the lack of the specific heat below 2 K. From the analysis, one can conclude Zr\(_2\)Ru\(_3\)Si\(_4\) not to be an isotropic single-gap superconductor, but likely to be a two-gap or anisotropic superconductor.

Figure 3 shows the magnetic field dependence of the magnetization \( M \) below \( T_c \). The existence of the superconducting mixed state characterizes Zr\(_2\)Ru\(_3\)Si\(_4\) as a type-II superconductor. The magnetization is irreversible. This would be caused by defects and impurities in the sample; they trap magnetic flux through the sample. The inset shows the initial magnetization at low fields. The dotted line shows the perfect diamagnetization. Since the magnetization gradually deviates from the perfect diamagnetization line, the lower critical field \( H_{c2}(T) \) is difficult to determine correctly. Here, we note only that \( H_{c2}(0) \) is approximately \( 1 \times 10^2 \) Oe.

Temperature dependence of the upper critical field \( H_{c2}(T) \) is shown in figure 4. \( H_{c2}(T) \) is estimated based on the electrical resistivity \( \rho(T) \) and heat capacity \( C_{\text{ELEC}}(T) \) under the magnetic field. The electrical resistivity under the magnetic field up to 80 kOe is illustrated in the inset. The transition temperature is suppressed by the field. \( H_{c2}^p(T) \) was determined by 10, 50 and 90% of the normal state resistivity before the transition. \( H_{c2}^p(T) \) was taken from the centre of the specific heat jump in figure 2(c). The curvature between \( H_{c2}^p(T) \) and \( H_{c2}^c(T) \) displays a small difference. This would be because resistivity measurements are easily affected by grain boundaries compared to capacity measurements. \( H_{c2}(T) \) shows the sizeable positive curvature near \( T_c \). The gradient of the curve in the vicinity of \( T_c \), \( -dH_{c2}^p/dT \), is 10 kOe K\(^{-1}\). The Werthamer–Helfand–Hohenberg (WHH) curves with clean and dirty limit [32], based on the isotropic single-gap model, are plotted by the dashed–dotted and broken lines, respectively. In conventional superconductors, \( H_{c2}(T) \) is well described by WHH curves. It is clear that the observed data are inconsistent with both of the WHH curves, indicating that the superconducting gap symmetry of Zr\(_2\)Ru\(_3\)Si\(_4\) is not an isotropic s-wave. If \( H_{c2}^{50\%} \) is extrapolated linearly to 0 K, \( H_{c2}(0) \) is about \( 1 \times 10^2 \) kOe. The coherence length \( \xi \) estimated by the relation \( \xi = [\phi_0 / 2\pi H_{c2}(0)]^{1/2} \) is 6 nm, where \( \phi_0 \) is the flux quantum.

Figure 5(a) shows the band structure for Zr\(_2\)Ru\(_3\)Si\(_4\) obtained by electronic structure calculations in an energy window near Fermi energy \( E_F \). Figure 5(b) illustrates the DOS of Zr\(_2\)Ru\(_3\)Si\(_4\) in the unit of states eV\(^{-1}\) formula unit (f.u.)\(^{-1}\). In both the figures, \( E_F \) is set to 0 eV. The density of states at \( E_F \) is \( N(E_F) = 3.2 \) states eV\(^{-1}\) f.u.\(^{-1}\). The partial DOS of each element is also shown in figure 5(b). There is little difference between sites in each atom (not shown), indicating a highly itinerant electron character of Zr\(_2\)Ru\(_3\)Si\(_4\). The partial DOS indicates that the bands near \( E_F \) consist of Ru 4d, Zr 4d and Si 3p states. The electrons of all the three species of ions contribute to form the Fermi surfaces (FFs) and probably the superconductivity as well. In the lower bands from \(-6.5 \) to \(-0.5 \) eV, the Ru 4d state is relatively predominant. FFs plotted in the first Brillouin zone are illustrated in figure 5(b) [33]. The two electron FFs exist around M and Z points, and a hole FS around V point. The anisotropic FFs reflect the low-symmetric crystal structure of Zr\(_2\)Ru\(_3\)Si\(_4\).

Temperature dependence of the electrical resistivity under the pressure \( P = 0.2, 0.6, 1.1 \) and 1.7 GPa is shown...
by $T_c \sim 1.14 \langle \omega \rangle \exp \left\{ -1/(N(E_F)V) \right\}$, where $V$ is the pairing potential arising from the electron–phonon interaction. By the McMillan expression [34], $N(E_F)V = N(E_F)(\langle I^2 \rangle/M \langle \omega^2 \rangle)$, the relation becomes,

$$T_c \sim 1.14 \langle \omega \rangle \exp \left\{ -M \langle \omega^2 \rangle/N(E_F) \langle I^2 \rangle \right\},$$

where $\langle I^2 \rangle$ stands for the average square electronic matrix element, $\langle \omega^2 \rangle$ the average square phonon frequency, and $M$ the mass of the ion. $T_c$ is more affected by $\omega$ in the exponent term than in the coefficient term; an increase of $\omega$ results in a decrease of $T_c$. Therefore, by the representation, the pressure dependence result indicates that the pressure-induced stiffening of the lattice vibration spectrum dominates over the minor changes in the electronic properties in Zr$_2$Ru$_3$Si$_4$ [35, 36]. Additionally, the result suggests that the contraction of the volume is disadvantageous to the superconductivity of Zr$_2$Ru$_3$Si$_4$. This may explain why Hf$_2$Ru$_3$Si$_4$ is not a superconductor; the cell volume of Hf$_2$Ru$_3$Si$_4$ is 1% smaller than that of Zr$_2$Ru$_3$Si$_4$ [10].

4. Discussion

The zero resistivity, magnetic flux expulsion and heat capacity jump clearly demonstrate superconductivity of Zr$_2$Ru$_3$Si$_4$ below $T = 5.5$ K. In addition, the magnetic field dependence of the magnetization suggests that it is type-II superconductivity. This can be verified numerically with the Ginzburg–Landau parameter $\kappa$. $\kappa$ is estimated by the relation $H_{c2}(0)/H_{c1}(0) = 2\kappa^2/\ln \kappa$. Employing the approximate values of $H_{c2}(0) = 1 \times 10^5$ kOe and $H_{c1}(0) = 1 \times 10^6$ Oe gives $\kappa = 5 \times 10^3$. The fact that $\kappa$ is rather larger than $1/\sqrt{2}$ also supports the type-II superconductivity.

An empirical electron–phonon interaction strength $\lambda_M$ is estimated by the McMillan formula [34],

$$\lambda_M = \frac{1.04 + \mu^* \ln(\theta_D/1.45T_c)}{(1-0.62\mu^*) \ln(\theta_D/1.45T_c) - 1.04},$$

in figure 6. $T_c$ is decreased with increasing the pressure, as seen in the majority of the superconductors. The inset shows the pressure dependence of $T_c$. $T_c$ is determined by the intersection of the extrapolated resistivity lines above and below the upper side of the transition. The pressure dependence of $T_c$ was fitted with a quadratic function and gives $T_c = -0.16P^2 + 0.06P + 6.02$. According to the BCS theory, a relation between $T_c$, typical phonon energy $\langle \omega \rangle$ and the interaction strength $N(E_F)V$ is given
where the repulsive screened Coulomb part $\mu^*$ is set to 0.13. This yields $\lambda_M = 0.77$, characterizing $\text{Zr}_2\text{Ru}_3\text{Si}_4$ as an intermediate-coupling superconductor. On the other hand, $N(E_F)$ and $\gamma$ give $\lambda_N = 0.74$ by the relation $(1 + \lambda_N) = 3\gamma/(\pi^2 k_B^2)N(E_F)$; this is consistent with $\lambda_M$.

Additionally, two results imply that the superconducting gap is not an isotropic single-gap. One is the deviation of the electronic heat capacity from the BCS s-wave structure calculation, and H Mamiya, H Kitaguchi and H Kitazawa for lending us their PPMS and MPMS. This work was supported by the Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST), Japan.

5. Conclusions

In this study, superconducting properties of the polycrystalline $\text{Zr}_2\text{Ru}_3\text{Si}_4$ were investigated by measuring electrical resistivity, magnetization and heat capacity. Superconducting transition of $T_c = 5.5$ K was confirmed. $\text{Zr}_2\text{Ru}_3\text{Si}_4$ was found to be a type-II and intermediate-coupling superconductor. Interestingly, the deviation of the heat capacity from the BCS isotropic s-wave model below $1/2T_c$. The other is the positive curvature of $H_{c2}(T)$ near $T_c$. Similar behaviours were observed in MgB$_2$ [30], YNi$_2$B$_2$C [37], Lu$_2$Fe$_3$Si$_5$ [4], Sc$_3$Ir$_4$Si$_{10}$ [4], $\beta$-Bi$_2$Pd [38], La$_3$Pd$_4$Si$_4$ [39], etc; they are considered to be multi-gap superconductors. Except for the multi-gap scenario, the positive curvature of $H_{c2}(T)$ is suggested theoretically according to an anisotropic gap [40], quasi-2D fluctuations [41], quantum critical point scenario [42] and bipolaronic scenario [43]. In $\text{Zr}_2\text{Ru}_3\text{Si}_4$, a multi-gap or anisotropic gap scenario would be preferable, since $\text{Zr}_2\text{Ru}_3\text{Si}_4$ has anisotropic Fermi surfaces. For further understanding of the superconducting gap symmetry of $\text{Zr}_2\text{Ru}_3\text{Si}_4$, $H_{c2}(T)$ and heat capacity measurements on a single crystal and in lower temperatures below $T = 2$ K are required.

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References

[1] Braun H F 1984 J. Less-Common Met. 100 105
[2] Steglich F, Aarts J, Bredl C D, Liece W, Meschede D, Franz W and Schafer H 1979 Phys. Rev. Lett. 43 1892
[3] Braun H F 1980 Phys. Lett. A 75 386
[4] Tamegai T, Nakajima Y, Nakagawa T, Li G and Harima H 2008 Sci. Technol. Adv. Mater. 9 044206
[5] Braun H F and Segre C U 1980 Solid State Commun. 35 735
[6] Klepp K and Parthé E 1982 Acta Crystallogr. B 38 1105
[7] Evers J, Oehlinger G, Weiss A and Probst C 1984 Solid State Commun. 50 61
[8] Kneidinger F, Michor H, Sidorenko A, Bauer E, Zeiringer I, Rogl P, Blasch-Schnenner C, Keith D and Podloucky R 2013 Phys. Rev. B 88 104508
[9] Johnson V and Jeitschko W 1972 J. Solid State Chem. 4 123
[10] Chabot B, Parthé E and Braun H F 1985 Acta Crystallogr. C 41 1148
[11] Barz H, Ku H C, Meisner G P, Fisk Z and Matthias B T 1980 Proc. Natl Acad. Sci. USA 77 3132
[12] Zhong W X, Chevalier B, Etourneau J and Hagenmuller P 1986 Solid State Commun. 59 839
[13] Shiratori I, Tachi K, Takeda K, Todo S, Yagi T and Kanoda K 1995 Phys. Rev. B 52 6197
[14] Braun H F, Donze P and Chabot B 1986 Verh. Dtsch. Phys. Ges. 21 1452
[15] Brown H F and Müller M 1998 Superconductors: Transition Temperatures and Characterization of Elements, Alloys and Compounds, Se... Ti (Landolt–Börnstein, Group III Condensed Matter vol 21d) (Berlin: Springer) (Si (Silicon)) pp 69–86
[16] Chabot B and Parthé E 1985 Acta Crystallogr. B 41 213
[17] Schappacher F M, Katoch K and Pöttgen R 2007 J. Solid State Chem. 180 186
[18] Eremets M I 1996 High-pressure experimental methods Oxford Science Publications (Oxford: Oxford University Press)
[19] Bireckoven B and Wittig J 1988 J. Phys. E: Sci. Instrum. 21 841
[20] Vanderbilt D 1990 Phys. Rev. B 41 7892
[21] Giannozzi P et al 2009 J. Phys.: Condens. Matter 21 395502
[22] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[23] Monkhorst H J and Pack J D 1976 Phys. Rev. B 13 5188
[24] Buschinger B, Greibel C, Diehl J, Weiden M, Guth W, Wildbrett A, Horn S and Steglich F 1997 J. Alloys Compounds 256 57
[25] Gottlieb U, Laborde O, Rouault A and Madar R 1993 Appl. Surf. Sci. 73 243
[26] Woodard D W and Cody G D 1964 Phys. Rev. 136 A166
[27] Fisk Z and Webb G W 1976 Phys. Rev. Lett. 36 1084
[28] Allen P B, Pickett W E, Ho K M and Cohen M L 1978 Phys. Rev. Lett. 40 1532
[29] Padamsee H, Neighbor J E and Shiffman C A 1973 J. Low Temp. Phys. 12 387
[30] Bouquet F, Wang Y, Fisher R A, Hinks D G, Jorgensen J D, Junod A and Phillips N E 2001 Europhys. Lett. 56 856
[31] Huang C L, Lin J Y, Sun C P, Lee T K, Kim J D, Choi E M, Lee S I and Yang H D 2006 Phys. Rev. B 174 288
[32] Kokalj A 2003 Comput. Mater. Sci. 25 155
[33] McMillan W L 1968 Phys. Rev. 167 331
[34] Hopfield J J 1971 Physica 55 41
[35] Schlüflig J S 2007 Handbook of High-Temperature Superconductivity: Theory and Experiment (New York: Springer) chapter (High-Pressure Effects) pp 427–57
[36] Shulga S V, Drechsler S L, Fuchs G, Müller K H, Winzer K, Heinecke M and Krug K 1998 Phys. Rev. Lett. 80 1730
[37] Imai Y, Nabeshima F, Yoshinaka T, Miyatani K, Kondo R, Komiya S, Tsukada I and Maeda A 2012 J. Phys. Soc. Japan 81 113708
[38] Kneidinger F, Michor H, Bauer E, Gribanov A, Lipatov A, Sereni Y S J and Rogl P 2013 Phys. Rev. B 88 024423
[39] Metlushko V, Welp U, Koshelev A, Aranson I, Crabtree G W, van Canpenfield P C 1997 Phys. Rev. Lett. 79 1738
[40] Boccelli S R 1995 Phys. Rev. Lett. 75 1376
[41] Kotliar G and Varma C M 1996 Phys. Rev. Lett. 77 2296
[42] Alexandrov A S 1993 Phys. Rev. B 48 10571