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2001 J. Phys.: Condens. Matter 13 L97

(http://iopscience.iop.org/0953-8984/13/4/105)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **13** (2001) L97–L103 www.iop.org/Journals/cm PII: S0953-8984(01)17770-2

LETTER TO THE EDITOR

Effects of misfit stresses on high-T_C superconductivity in thin-film cuprates

I A Ovid'ko

Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vasilyevsky Ostrov, St Petersburg 199178, Russia

E-mail: ovidko@def.ipme.ru

Received 5 October 2000, in final form 20 November 2000

Abstract

Effects of misfit stresses on the high-transition-temperature superconducting properties of thin-film cuprates are predicted and theoretically examined. A substantial enhancement of the critical transition temperature is predicted for $YBa_2Cu_3O_{7-y}$ and $Bi_2Sr_2CaCu_2O_x$ superconducting films, which is induced by misfit stresses generated at interphase boundaries with special crystallography and large misfit. The influence of misfit stresses on the structure and the transport properties of low-angle tilt boundaries in superconducting thin-film cuprates is theoretically analysed.

1. Introduction

The high-transition-temperature (T_C) superconducting properties of cuprates are strongly influenced by mechanical stresses. Experiments [1, 2] have shown a substantial increase of T_C under external-load-induced hydrostatic pressure, from several degrees for $Bi_2Sr_2CaCu_2O_x$ to about 20 K for $HgBa_2Ca_2Cu_3O_{8+z}$ superconductors. The experimentally observed drastic reduction of the critical current density J_c across grain boundaries (see, e.g., [3–6]) and structural transformations of grain boundaries [7] can be effectively treated as occurring due to stress fields induced by grain boundary dislocations [8–12]. In general, stresses created by grain boundary and lattice dislocations are also capable of causing enhancement of high-T_C superconductivity in the vicinities of dislocations [13].

In thin-film superconductors there are internal stress-field sources which are different from grain boundaries and lattice dislocations. In particular, such sources include interphase (film/substrate) boundaries that induce misfit stresses due to mismatch between crystal lattice parameters of films and substrates. Misfit stresses are well known to affect both the structure and the behaviour of conventional (non-superconducting) films; see, e.g., [14–21]. Also, recently, the doubling of the critical temperature T_C in LaSrCuO superconducting thin films due to compressive misfit stresses has been reported [22]. This leads us to think that misfit stresses created by interphase boundaries are capable of strongly affecting the high-T_C superconducting properties of thin-film cuprates. The main aim of this letter is to predict and theoretically

0953-8984/01/040097+07$30.00

examine (in the first approximation) the following two effects of misfit stresses on high-T_C superconductivity in thin-film cuprates: increase of T_C in $YBa_2Cu_3O_{7-y}$ and $Bi_2Sr_2CaCu_2O_x$ thin films due to misfit stresses; and increase of J_c across low-angle tilt boundaries due to misfit-stress-induced structural changes of such boundaries.

2. The enhancement of the transition temperature T_C for superconducting $YBa_2Cu_3O_{7-y}$ and $Bi_2Sr_2CaCu_2O_x$ thin films due to misfit stresses

The experimentally observed sensitivity of T_C to dilatation stresses in optimally doped $YBa_2Cu_3O_{7-y}$ single crystals is characterized by the pressure derivatives $\mathrm{d}T_C/\mathrm{d}p_a = -1.9$–$2\ \mathrm{K\ GPa^{-1}}$, $\mathrm{d}T_C/\mathrm{d}p_b = 1.9$–$2.2\ \mathrm{K\ GPa^{-1}}$ and $\mathrm{d}T_C/\mathrm{d}p_c = -0$–$0.3\ \mathrm{K\ GPa^{-1}}$ [23], where the subscript of p_l denotes the crystallographic axis. The characteristic values of the pressure derivatives of $Bi_2Sr_2CaCu_2O_x$ single crystals are as follows: $\mathrm{d}T_C/\mathrm{d}p_a = 1.6\ \mathrm{K\ GPa^{-1}}$, $\mathrm{d}T_C/\mathrm{d}p_b = 2\ \mathrm{K\ GPa^{-1}}$ and $\mathrm{d}T_C/\mathrm{d}p_c = -2.8\ \mathrm{K\ GPa^{-1}}$ (see the experimental data in [24]). In view of these values of $\mathrm{d}T_C/\mathrm{d}p_l$, we think that coherent interphase boundaries induce in-plane misfit stresses that are capable of effectively enhancing T_C for single-crystalline superconducting $YBa_2Cu_3O_{7-x}$ and $Bi_2Sr_2CaCu_2O_x$ films. More precisely, T_C-enhancement is expected in $YBa_2Cu_3O_{7-x}$ films due to misfit stresses created by coherent interphase boundaries with (a, c) and (b, c) crystallographic planes, which are characterized by the sets of pressure derivatives ($\mathrm{d}T_C/\mathrm{d}p_a = -1.9$–$2\ \mathrm{K\ GPa^{-1}}$, $\mathrm{d}T_C/\mathrm{d}p_c = -0$–$0.3\ \mathrm{K\ GPa^{-1}}$) and ($\mathrm{d}T_C/\mathrm{d}p_b = 1.9$–$2.2\ \mathrm{K\ GPa^{-1}}$, $\mathrm{d}T_C/\mathrm{d}p_c = -0$–$0.3\ \mathrm{K\ GPa^{-1}}$), respectively. Also, T_C-enhancement can effectively occur in $Bi_2Sr_2CaCu_2O_x$ superconducting films due to misfit stresses generated at the interphase boundary with the (a, b) plane, in which case the sensitivity of T_C to the stresses is specified by the set of pressure derivatives ($\mathrm{d}T_C/\mathrm{d}p_a = 1.6\ \mathrm{K\ GPa^{-1}}$, $\mathrm{d}T_C/\mathrm{d}p_b = 2\ \mathrm{K\ GPa^{-1}}$).

Let us consider the dependence of the misfit-stress-induced change ΔT_C of the transition temperature on the misfit parameters of superconducting film/substrate systems. Let f_a, f_b and f_c be the misfit parameters defined, according to the theory of interphase boundaries [14, 15], as follows:

$$f_a = \frac{a_a - a}{a_a} \qquad f_b = \frac{a_b - b}{a_b} \qquad f_c = \frac{a_c - c}{a_c} \tag{1}$$

where a, b and c are the crystal lattice parameters of a superconducting film along the crystallographic a-, b- and c-axes, respectively, and a_a, a_b and a_c are the crystal lattice parameters of a substrate along the crystallographic a-, b- and c-axes, respectively. For a coherent interphase boundary (between a thin film and a thick substrate) in the (i, k) plane (where $i, k = a, b, c$ and $i \neq k$), the non-zero components of the misfit stress tensor in the film are given as [14]

$$\sigma_{ii} = -E(f_i + \nu f_k)/(1 - \nu^2) \qquad \sigma_{kk} = -E(f_k + \nu f_i)/(1 - \nu^2) \tag{2}$$

where E denotes Young modulus and ν the Poisson ratio. In the situation discussed, $\sigma_{ii} = p_i$ and $\sigma_{kk} = p_k$. As a corollary, we find that the change $(\Delta T_C)_{i,k}$ of the transition temperature of the superconducting film due to misfit stresses generated at the interphase boundary with the (i, k) plane depends on the misfit parameters f_i and f_k as follows:

$$(\Delta T_C)_{i,k} = -(\mathrm{d}T_C/\mathrm{d}p_i)\frac{E(f_i + \nu f_k)}{(1 - \nu^2)} - (\mathrm{d}T_C/\mathrm{d}p_k)\frac{E(f_k + \nu f_i)}{(1 - \nu^2)}. \tag{3}$$

With the misfit parameters f_a, f_b and f_c assumed to be identical ($f_a = f_b = f_c = f$), the dependences of $(\Delta T_C)_{i,k}$ on f, given by formula (3), are presented in figure 1 for the following cases: $(\Delta T_C)_{a,b}$ for the superconducting $Bi_2Sr_2CaCu_2O_x$ film (line 1 in figure 1); $(\Delta T_C)_{a,c}$ and

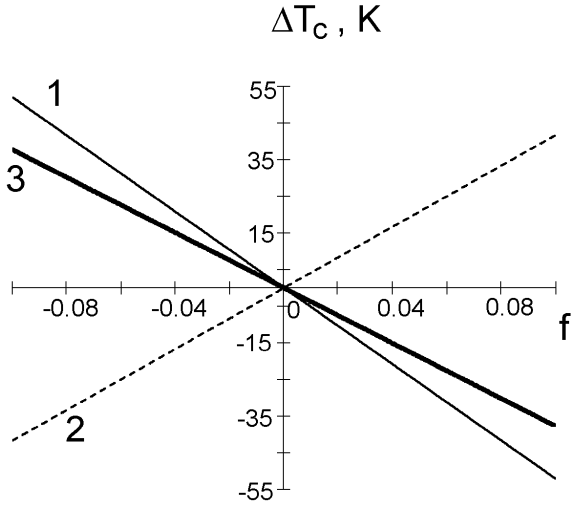

Figure 1. Dependences of ΔT_C on the misfit parameter f, for $Bi_2Sr_2CaCu_2O_x$ film with the interphase boundary in the (a, b) plane (line 1) and $YBa_2Cu_3O_{7-y}$ films with interphase boundaries in the (a, c) plane (dashed line 2) and the (b, c) plane (solid line 3).

$(\Delta T_C)_{b,c}$ for the superconducting $YBa_2Cu_3O_{7-x}$ film (lines 2 and 3, respectively, in figure 1). (In the calculation of the dependences shown in figure 1 we have used values of E and ν given by experiments: $E = 81$ GPa and $\nu \approx 0.44$ for $Bi_2Sr_2CaCu_2O_x$ superconductors [25]; $E \approx 148$ GPa and $\nu \approx 0.255$ for $YBa_2Cu_3O_{7-x}$ superconductors [26].) The dependences (figure 1) indicate that the misfit stresses are capable of causing a substantial increase of the transition temperature T_C for $Bi_2Sr_2CaCu_2O_x$ and $YBa_2Cu_3O_{7-y}$ superconducting films with coherent interphase boundaries.

It should be noted that the above-discussed effect of misfit stresses occurs most effectively if the cuprate film thickness is optimum. This thickness is a compromise between the generation of misfit dislocations (that compensate, in part, for misfit stresses [14–19, 21]) and minimizing the T_C-reduction observed [27] for ultrathin films. To exhibit a substantial enhancement of T_C, a thin-film cuprate should be characterized by the optimum thickness, large misfit parameters and a special crystallography of the interphase boundary. These are rather restrictive conditions for real film/substrate systems. In particular, as misfit parameters grow, the critical film thickness h_c (at which generation of misfit dislocations is energetically favourable) decreases [14–16]. Also, the deposition of cuprate films onto substrate materials in the case of large misfit requires a previous coating with an adequate buffer layer which provides for epitaxial growth by reducing the lattice mismatch between substrate and film [28]. The above can explain the fact that, to the author's knowledge, up to now, T_C-enhancement due to misfit stresses has not been experimentally detected for YBaCuO and BiSrCaCuO films.

3. The effect of misfit stresses on the structure and transport properties of low-angle tilt boundaries in polycrystalline superconducting films

As shown by [21, 29, 30], grain boundary dislocations in polycrystalline films can play a role as misfit defects compensating, in part, for misfit stresses generated at interphase boundaries. In doing so, misfit stresses influence the grain boundary structures which, therefore, are different from those in bulk materials. Let us consider this effect of misfit stresses for the example of a low-angle tilt boundary composed of lattice dislocations of the edge type. Let the grain boundary dislocations be parallel with the interphase boundary plane and be periodically arranged in some initial state of the as-synthesized polycrystalline film (figure 2(a)); the dislocations provide misorientation of the adjacent grains of the film and do not contribute to the relaxation of the misfit stresses. In particular, this means that the misorientation θ_1 of the grain boundary in its initial state is consistent the with misorientations, θ' and θ'', of the interphase boundary fragments adjacent to the grain boundary (figure 2(a)). That is, $\theta_1 = -\theta' - \theta''$.

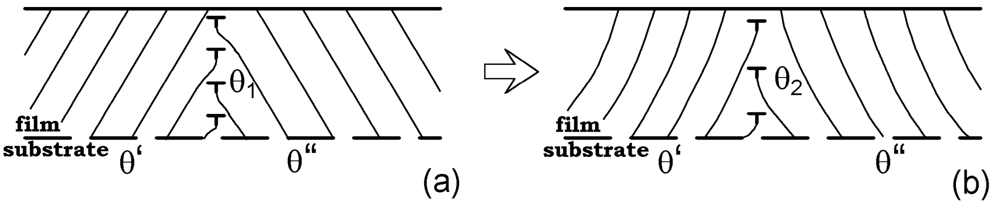

Figure 2. The transformation of the low-angle boundary structure from the initial state (a) with misorientation θ_1 to the final state (b) with misorientation θ_2 ($<\theta_1$).

Let us consider a transformation of the low-angle boundary from its initial state with misorientation θ_1 (figure 2(a)) into a state with misorientation θ_2 ($<\theta_1$) (figure 2(b)). The transformation occurs via climbing of m ($m \geqslant 1$) grain boundary dislocations towards the film free surface, where these dislocations disappear. Due to the transformation, the low-angle boundary acquires an 'uncompensated' dislocation density associated with the difference $\Delta\theta = \theta_2 - \theta_1$ between its misorientations in the final and initial states. The low-angle boundary with the uncompensated dislocation density creates stress fields which compensate, in part, for misfit stresses [21, 29, 30]. As a corollary, the transformation of the boundary structure (figure 2) is driven by a release of misfit stresses in the film.

Let us examine the energetic characteristics of the transformation (figure 2) with the assumptions that: (i) the film contains identical low-angle boundaries periodically spaced along the interphase boundary; and (ii) dislocations that compose the low-angle boundaries in their final state (after the transformation) are arranged periodically. In the framework of the suggested approximation, the transformation of the low-angle boundary dislocation structures (figure 2) is equivalent to the formation of a periodic row of misfit disclinations (rotational defects each characterized by a strength $\omega = \theta_2 - \theta_1 < 0$) at the interphase boundary, whose stress fields compensate, in part, for the misfit stresses; for more details, see [29, 30]. In the following, for definiteness and for the sake of simplicity, we restrict our consideration to the case with the one-dimensional misfit parameter

$$\tilde{f} = \frac{a_s - a_f}{a_s} > 0$$

where a_s and a_f are the crystal lattice parameters of the substrate and the film, respectively. Also, the thin film and the (model) semi-infinite substrate are assumed to be isotropic and characterized by the same values of the shear strength G and the same values of the Poisson ratio ν. In these circumstances, following calculations [29], the energy-density change ΔE^{ω} related to the formation of the misfit disclination row is obtained as follows:

$$\Delta E^{\omega} = \frac{G\omega^2 l}{4\pi(1-\nu)}\Phi(h/l) - \frac{G|\omega|\tilde{f}h^2}{(1-\nu)l} \tag{4}$$

where

$$\Phi = \int_{-\tilde{h}}^{0} \left[\frac{1}{2} \ln \frac{\cosh 2\pi(\tilde{x}+\tilde{h}) - 1}{\cosh 2\pi(\tilde{x}-\tilde{h}) - 1} + \pi(\tilde{x}+\tilde{h}) \frac{\sinh 2\pi(\tilde{x}+\tilde{h})}{\cosh 2\pi(\tilde{x}+\tilde{h}) - 1} - \pi(\tilde{x}+3\tilde{h}) \frac{\sinh 2\pi(\tilde{x}-\tilde{h})}{\cosh 2\pi(\tilde{x}-\tilde{h}) - 1} - 4\pi^2 \tilde{x}\tilde{h} \frac{1}{\cosh 2\pi(\tilde{x}-\tilde{h}) - 1} \right] (\tilde{x}+\tilde{h})\, d\tilde{x}. \quad (5)$$

Here h denotes the film thickness, l the distance between neighbouring misfit disclinations and $\tilde{h} = h/l$.

The energy density $\Delta E^b \approx mGb^2/4\pi(1-\nu)l$ characterizes the core energy density of m dislocations with Burgers vectors $\boldsymbol{b}$, which disappeared during the transformations of the grain boundary structures (figure 2). From the geometry of a transformed low-angle boundary, we have the following relationship between its parameters: $mb \approx h|\omega|$ at $|\omega| \ll 1$. With this relationship, and with ΔE^{ω} (given by formulae (4) and (5)) and ΔE^b taken into account, we find the energy-density change ΔE related to the transformation (figure 2) to be given as

$$\Delta E = E_2 - E_1 = \frac{Gb}{4\pi(1-\nu)} \left[\frac{m^2 bl}{h^2} \Phi(h/l) - \frac{4\pi \tilde{f} mh}{l} - \frac{mb}{l} \right] \quad (6)$$

where E_1 (E_2) is the energy density of the film with the low-angle boundary in its initial (final) state. Over the wide ranges of parameters characterizing the film, $\Delta E < 0$ (see, for instance, the dependences of ΔE on m in figure 3); that is, the misfit-stress-induced transformation (figure 2) is energetically favourable.

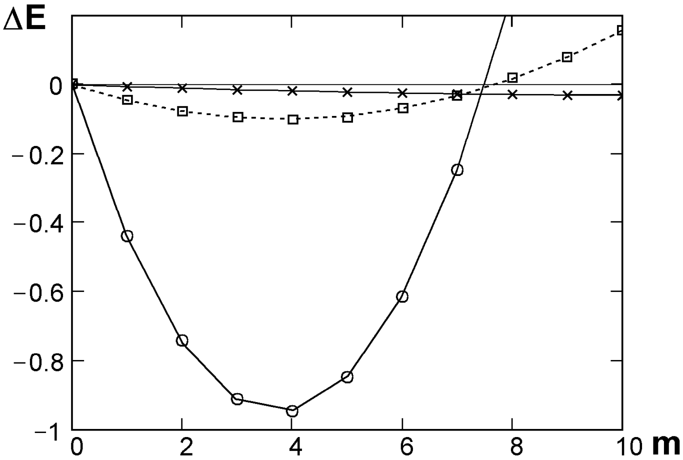

Figure 3. The dependence of ΔE (in units of $Gb/4\pi(1-\nu)$) on the number m of misfit dislocations removed from a low-angle boundary, for $b = 0.4$ nm, $\tilde{f} = 10^{-2}$ and: (i) $l = 1000$ nm, $h = 100$ nm (crosses); (ii) $l = 100$ nm, $h = 1000$ nm (open circles); (iii) $l = 100$ nm, $h = 100$ nm (open boxes).

On the basis of experimental data [5, 6], it is tentatively suggested that the critical current density across [001] tilt boundaries in $YBa_2Cu_3O_{7-y}$ superconductors at the temperature $T = 4.2$ K depends on the boundary misorientation θ as follows:

$$J_c(\theta) = J_{bulk} \exp[-\theta/\theta_0] \quad (7)$$

where $\theta_0 \approx 6.3°$, the typical bulk current density $J_{bulk} \approx 2 \times 10^7$ A cm^{-2} and θ ranges from 0° to 45°. Owing to the highly non-linear character of the dependence $J_c(\theta)$ given by formula (7), we find that the misfit-stress-induced transformation of the low-angle boundary structures (figure 2) enhances the critical current density across low-angle tilt boundaries in superconducting films. The ratio of the critical current density ($J_c(\theta_2)$) across the low-angle boundary in its final state to that ($J_c(\theta_1)$) in its initial state is given as

$$J_c(\theta_2)/J_c(\theta_1) = \exp[(\theta_1 - \theta_2)/\theta_0] > 1 \qquad \text{for } \theta_2 < \theta_1.$$

The misfit-stress-driven transformations of tilt boundary structures (figure 2) require grain boundary dislocations to climb towards the film free surface, in which case the dislocations should overcome some energetic barriers related to emission or absorption of point defects at the dislocation cores [31]. Pressure and thermal treatment are capable of enhancing the climbing of dislocations and, therefore, according to our model, increasing J_c. In this context, recent experimental data [32] on a significant enhancement of J_c achieved by hot pressing in Bi-2223/Ag multifilamentary tapes can be seen as supporting the model suggested in this letter.

4. Summary

To summarize, according to results of our theoretical analysis, misfit stresses are capable of enhancing such important characteristics of high-T_C superconducting thin-film cuprates as the transition temperature T_C and the critical current density J_c. This potentially allows one to use technologically controlled parameters (misfit parameters, crystallography of interphase boundary, film thickness) of film/substrate systems in the synthesis and design of high-T_C superconducting films with enhanced functional properties.

This work was supported, in part, by the Office of US Naval Research (grant N00014-99-1-0896) and the Russian Foundation of Basic Research (grant 98-02-16075).

References

[1] Chu C W, Gao L, Chen F, Huang Z J, Meng R L and Xue Y Y 1993 *Nature* **365** 323–5
[2] Nunez-Regueiro M, Tholence J-L, Antipov E V, Capponi J-J and Marezio M 1993 *Science* **262** 97–9
[3] Dimos D, Chaudhari P, Mannhart J and LeGoues F K 1988 *Phys. Rev. Lett.* **61** 219–22
[4] Dimos D, Chaudhari P and Mannhart J 1990 *Phys. Rev.* B **41** 4038–49
[5] Ivanov Z G, Nilsson P-Å, Winkler D, Alarco J A, Claeson T, Stepantsov E A and Tzalenchuk A Ya 1991 *Appl. Phys. Lett.* **59** 3030–2
[6] Heinig N F, Redwing R D, Tsu I F, Gurevich A, Nordman J E, Babcock S E and Larbalestier D C 1996 *Appl. Phys. Lett.* **69** 577–9
[7] Chisholm M F and Smith D A 1989 *Phil. Mag.* A **59** 181–91
[8] Chisholm M F and Pennycook S J 1991 *Nature* **351** 47–9
[9] Agassi D, Pande C S and Masumura R A 1995 *Phys. Rev.* B **52** 16 237–49
[10] Alarco J A and Olsson E 1995 *Phys. Rev.* B **52** 13 625–30
[11] Gutkin M Yu and Ovid'ko I A 2001 *Phys. Rev.* **63** at press
[12] Gurevich A and Pashitskii E A 1998 *Phys. Rev.* B **57** 13 878–93
[13] Gurevich A and Pashitskii E A 1997 *Phys. Rev.* B **56** 6213-25
[14] Tkhorik Yu A and Khazan L S 1983 *Plastic Deformation and Misfit Dislocations in Heteroepitaxial Systems* (Kiev: Naukova Dumka) (in Russian)
[15] Jain S C, Harker A H and Cowley R A 1997 *Phil. Mag.* A **75** 1461–515
[16] Fitzerald E A 1991 *Mater. Sci. Rep.* **7** 87–142
[17] Rocket A and Kiely C J 1991 *Phys. Rev.* B **44** 1154–62
[18] van der Merve J H 1991 *Crit. Rev. Solid State Mater. Sci.* **17** 187–209
[19] Willis J R, Jain S C and Ballough R 1990 *Phil. Mag.* A **62** 115–9
[20] Gutkin M Yu and Ovid'ko I A 1999 *J. Phys.: Condens. Matter* **11** 8607–16
[21] Ovid'ko I A 2000 *Nanostructured Films and Coatings (NATO Science Series)* ed G M Chow, I A Ovid'ko and T Tsakalakos (Dordrecht: Kluwer) pp 231–46

[22] Locquet J-P, Perret J, Fompeyrine J, Mächler, Seo J W and Van Tendeloo G 1998 *Nature* **394** 453–8
[23] Welp U, Grimsditch M, Flesher S, Nessler W, Veal B and Grabtree G W 1994 *J. Supercond.* **7** 159–65
[24] Meingast C, Junod A and Walker E 1996 *Physica* C **272** 106–12
[25] Belomestnykh V N, Khazanov O L, Bush A A and Sirotkin V P 1990 *Supercond.: Phys., Chem., Tech.* **3** 221–4 (in Russian)
[26] Ledbetter H M, Kim S A, Goldfarb R B and Togano K 1989 *Phys. Rev.* B **39** 9689–92
[27] Triscone J-M, Fisher O, Brunner O, Antonazza L, Kent A D and Karkut M G 1990 *Phys. Rev. Lett.* **64** 804–7
[28] Woerdenweber R 1999 *Supercond. Sci. Technol.* **12** R86–102
[29] Kolesnikova A L, Ovid'ko I A and Romanov A E 2001 *Solid State Phenom.* at press
[30] Ovid'ko I A 1999 *J. Phys.: Condens. Matter* **11** 6521–7
[31] Hirth J P and Lothe J 1968 *Theory of Dislocations* (New York: McGraw-Hill)
[32] Zeng R, Ye B, Horvat J, Guo Y C, Zeimetz B, Yang X F, Beales T P, Liu H K and Dou S X 1998 *Supercond. Sci. Technol.* **11** 1101–4