Solid State Communications 200 (2014) 17–21

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Study of the superconducting phase in silicene under biaxial tensile strain

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ARTICLE INFO

Article history:
Received 15 July 2014
Received in revised form
4 September 2014
Accepted 6 September 2014
by R. Merlin
Available online 16 September 2014

Keywords:
A. Superconductivity
A. Two-dimensional systems
A. Silicene
D. Thermodynamic properties

ABSTRACT

The electron-doped silicene under the influence of the biaxial tensile strain is predicted to be the phonon-mediated superconductor. By using the Eliashberg formalism, we investigate the thermodynamic properties of the superconducting silicene in the case when the tension is 5% and the electron doping equals $3.5 \times 10^{14}\ \mathrm{cm}^{-2}$. Under such conditions, silicene monolayer is expected to exhibit the highest superconducting transition temperature (T_C). In particular, based on the electron–phonon spectral function and assuming a wide range of the Coulomb pseudopotential values ($\mu^* \in \langle 0.1, 0.3 \rangle$) it is stated that the superconducting transition temperature decreases from 18.7 K to 11.6 K. Similar behavior is observed in the case of the zeroth temperature superconducting energy gap at the Fermi level: $2\Delta(0) \in \langle 6.68, 3.88 \rangle$ meV. Other thermodynamic parameters differ from the predictions of the Bardeen–Cooper–Schrieffer theory. In particular, the ratio of the energy gap to the critical temperature changes in the range from 4.14 to 3.87. The ratio of the specific heat jump to the specific heat in the normal state takes the values from 2.19 to 2.05, and the ratio of the critical temperature and specific heat in the normal state to the thermodynamic critical field increases from 0.143 to 0.155. It is also determined that the maximum value of the electron effective mass equals 2.11 of the electron band mass.

1. Introduction

Recent research in the field of nanotechnology has led to the synthesis and characterization of various two-dimensional materials [1]. The unique geometries of these novel structures are one of the main origins of their extraordinary physical and chemical properties [1,2]. Among different applications, the possibility of using such low-dimensional systems in the domain of nanoscale superconducting devices is of growing interest [3–5].

In this respect, the one-atom-thick two-dimensional form of carbon, known as graphene [6], attracted exceptional attention in recent years, when comparing to the other carbon allotropes [7–9]. However, various theoretical calculations demonstrate that the phonon-mediated superconductivity does not occur in the intrinsic graphene, due to the weak electron–phonon coupling constant [10–12]. This fact follows the case of graphite, where the induction of the superconducting phase is possible only via the chemical process know as intercalation [13].

In particular, it was suggested, by using the first-principle calculations, that the conventional superconducting state with notable high critical temperature (T_C) can be observed in the hole-doped graphene (a fully hydrogenated graphene) [14,15] or in the lithium-decorated graphene [13,16,17]. Due to these findings this direction of research can be considered as a promising and important one. However, the direct experimental evidences are still lacking.

Another noteworthy material for the superconducting nanoelectronic applications is silicene (the graphene-like monolayer of silicon) [18]. In general, the main advantage of this material is the fact that it combines some of the graphene intriguing properties and can be relatively easy to incorporate into the existing silicon-based electronics [19]. Moreover, the preliminary results on the synthesis of silicene are already available [20].

From the point of view of the superconducting properties, it is important that pristine silicene is characterized by the buckled structure, which distinguish it from the graphene and favors stronger electron–phonon coupling in this material [21]. Some theoretical works, using random-phase-approximation (RPA), have proposed possible singlet $d+id'$ chiral superconductivity in undoped bilayer silicene [22] or quantum phase transition to the triplet f-wave superconducting phase in doped silicene under a perpendicular external electric field [23]. Encouraging are also recent experimental results which suggest that the induction of the superconducting state in supported silicene may be possible [24].

On the other hand, latest theoretical investigations predict that the electron-doping and the influence of the biaxial tensile strain induce superconducting state characterized by the critical temperature much

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http://dx.doi.org/10.1016/j.ssc.2014.09.007
0038-1098/

above 10 K [21]. In particular, for the electron doping (n_e) equals 3.5×10^{14} cm^{-2} and tension of 5%, the analytical McMillan [25] formula gives $T_C \sim 17$ K. This outcome is promising and motivates our studies.

In the present paper, we concentrate ourselves on the analysis of the superconducting phase induced in silicene under the conditions mentioned above. In the considered case, the electron–phonon coupling constant exceeds the weak coupling limit ($\lambda > 0.5$ [26]). Due to this fact we conduct our calculations within the framework of the Eliashberg formalism [27], which allows us to calculate the thermodynamic properties of the superconducting phase at the quantitative level. Our calculations based on the electron–phonon spectral function $\alpha^2F(\omega)$ obtained in [21], by using the density functional theory within the local-density approximation. The numerical methods adopted in the present work based on the self-consistent iterative procedure presented in [16,28,29].

2. The numerical and analytical results

In order to compute all thermodynamic properties of interest, the Eliashberg equations are solved on the imaginary axis and in the mixed representation (defined simultaneously on the imaginary and real axis). The stability of the solutions in both cases is achieved in the temperature range from $T_0 = 1$ K to T_C, for the assumed 1100 Matsubara frequencies: $\omega_m \equiv (\pi/\beta)(2m-1)$, where $\beta \equiv 1/k_BT$, and k_B denotes the Boltzmann constant.

The Coulomb pseudopotential ($\mu^\star$) models the depairing interaction between the electrons and besides the Eliashberg function is the second input parameter in the Eliashberg equations. In fact there are two well-known experimental methods to determine $\mu^\star$. One is based on the isotope effect [25], second is based on the inversion of tunnelling data [30]. It should be emphasized that the isotope effect can be used only when a set of isotopes is available and the tunnelling experiments require strong or medium coupling superconductors in order to give sufficient structure in the current–voltage characteristic [31]. The physical value of Coulomb pseudopotential is hard to calculate from first-principles, so it is usually treated as a material-dependent adjustable parameter chosen, for examples within the framework of the Eliashberg formalism, to reproduce the experimental value of critical temperature [32]. However, due to absence of the experimental results for silicene, a wide range of the Coulomb pseudopotential values is taken into account: $\mu^\star \in \langle 0.1, 0.3\rangle$.

In Fig. 1(A), the superconducting order parameter on the imaginary axis for selected values of the temperature and the Coulomb pseudopotential is presented. The maximum value of the order parameter ($\Delta_{m=1}$) decreases with the growth of T and $\mu^\star$. This fact can be clearly observed in Fig. 1(B) where $\Delta_{m=1}(T)$ function is shown. On the basis of these results, we note that the $\Delta_{m=1}$ values can be well parameterized by the following formula:

$$\Delta_{m=1}(T,\mu^\star) = \Delta_{m=1}(\mu^\star)\sqrt{1-\left(\frac{T}{T_C}\right)^{\alpha}}, \tag{1}$$

where: $\Delta_{m=1}(\mu^\star) = 18.30(\mu^\star)^2 - 14.08\mu^\star + 4.51$ and the fitting parameter α is equal to 3.4.

The superconducting transition temperature is defined as the temperature at which the order parameter vanishes: $\Delta_{m=1}(T_C,\mu^\star) = 0$. In the case of silicene it is stated that T_C is high in the entire range of the Coulomb pseudopotential values. In particular, $T_C \in \langle 18.7, 11.6\rangle$ K for $\mu^\star \in \langle 0.1, 0.3\rangle$. It should be noted that the maximum value of the critical temperature for $\mu^\star = 0.1$ determined by us is significantly higher than the value predicted in the paper [21], where $[T_C]^{\max}_{\mu^\star=0.1} = 16.40$ K. This situation is caused by the fact that in the paper [21] the superconducting transition temperature was estimated by using McMillan formula [25]:

$$k_BT_C = \frac{\omega_{\ln}}{1.2}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^\star(1+0.62\lambda)}\right], \tag{2}$$

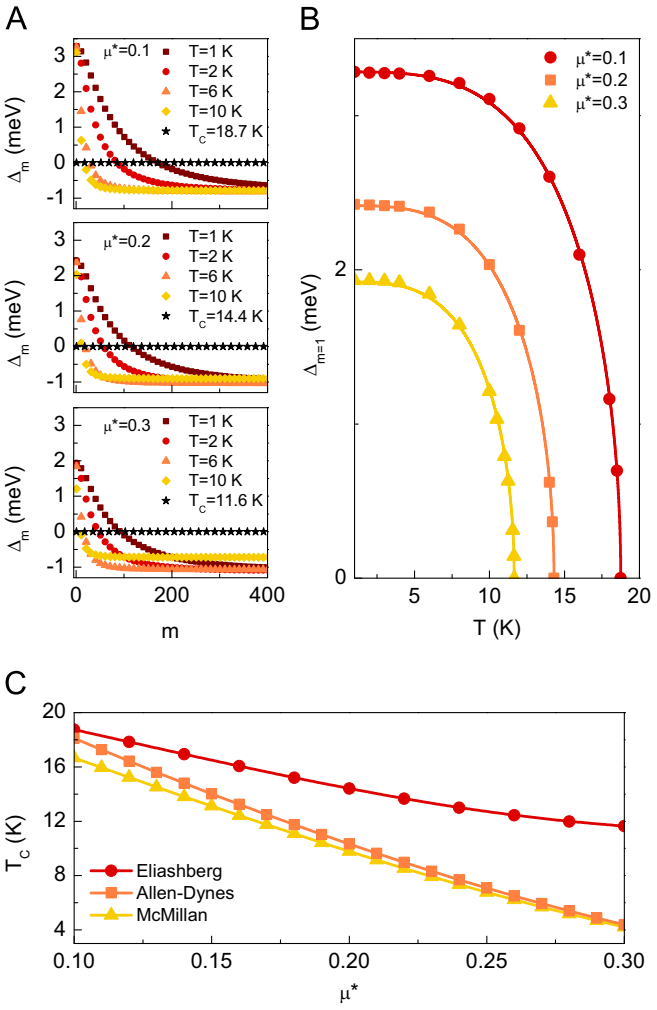

Fig. 1. (Color online) (A) The dependence of the order parameter on the number m for the selected temperatures and Coulomb pseudopotential values. (B) The full dependence of the maximum value of the order parameter on the temperature for selected $\mu^\star$. (C) The critical temperature as a function of the Coulomb pseudopotential. The circles correspond to the exact numerical solutions of the Eliashberg equations. The triangles and squares represent the results obtained using the Allen–Dynes and McMillan formula, respectively.

where $\omega_{\ln}$ is the logarithmic averaged phonon frequency and equals 18.52 meV for the tension of 5%.

A full dependence of T_C on $\mu^\star$ is plotted in Fig. 1(C). Presented results are obtained using the Eliashberg formalism, Allen–Dynes expression [30] and the McMillan formula [25]. It can be observed that the analytical results underestimate the critical temperature, especially for the high values of the Coulomb pseudopotential. Moreover, the Allen–Dynes expression much better predicts T_C than the McMillan formula.

In Fig. 2, we present the results for the wave function renormalization factor. The identical values of temperature and Coulomb pseudopotential as for the order parameter are chosen. It is found that the function $Z_{m=1}(T)$ increases together with the temperature and the Coulomb pseudopotential value.

The values of the function $Z_{m=1}(T,\mu^\star)$ can be estimated by the formula:

$$Z_{m=1}(T,\mu^\star) = Z_{m=1}(\mu^\star) + [Z_{m=1}(T_C) - Z_{m=1}(\mu^\star)]\left(\frac{T}{T_C}\right)^{\alpha}, \tag{3}$$