Second-order phase transition of silicon from a band insulator to metal induced by strong magnetic fields

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1. Introduction

Materials exhibit various properties in a magnetic field [1–3]. For example, Pauli paramagnetism and Landau diamagnetism that are described on the basis of the free electron model [1–3], Curie paramagnetism and Langevin diamagnetism that are described on the base of the localized electron model [1–3], de Haas–van Alphen (dHvA) effect [4, 5] and Shubnikov–de Haas effect [6] are observed in materials immersed in a magnetic field. The quantum Hall effect is observed in two-dimensional electron systems at low temperatures and under a strong magnetic field [7–9]. More recently, an anomalous value of the electron g-factor, which can be explained as the Rashba effect caused by the antisymmetric surface potential, is measured in graphene by the electron spin resonance experiments [10–12]. Furthermore, the giant magnetoresistance effect [13, 14] and the colossal magnetoresistance effect [15–18] are known as magnetic field-induced phenomena, and they have led to a field of spintronics [19]. The magnetic field-induced phase transition has been attracting much attention so far and have been actively studied in recent years [20–27]. Thus, various physical properties are observed in materials immersed in a magnetic field, which are different from those of materials in the zero magnetic field.

There are several kinds of methods to describe electronic states of materials immersed in a magnetic field. For example, the effective mass approximation method [1–3], the semiclassical approach [1–3] and the Hofstadter method [28] are widely used to describe electronic states of materials immersed in a magnetic field [29–32]. Recently, we developed the magnetic-field-containing relativistic tight-binding (MFRTB) method [33]. This method enables us to calculate the energy band structure for materials immersed in a magnetic field. The obtained energy band structure is described in the magnetic first Brillouin zone (BZ) and is sometimes called the magnetic energy band structure. By using the magnetic energy band structure obtained via the MFRTB method, it is shown that one can not only revisit the dHvA oscillation and magnetic breakdown phenomena, but also predict additional oscillation peaks of the magnetization [34, 35] that cannot be explained by the conventional Lifshitz–Kosevich formula [36].
In the MFRTB method [33] as well as in the Hofstadter method [28], the magnetic hopping integral is approximately given by the hopping integral in the absence of a magnetic field multiplied by the so-called Peierls phase factor. In order to increase the accuracy of the estimation of magnetic hopping integrals and to make the method applicable to materials immersed in a strong magnetic field, the nonperturbative MFRTB method has been developed [37, 38]. Although effects of the electron–electron interaction are not taken into consideration explicitly in the nonperturbative MFRTB method as well as the Hofstadter [28] and conventional MFRTB [33] methods, we have successfully obtained the approximate form of the magnetic hopping integral that is applicable to materials immersed in a strong magnetic field.

In this paper, we apply the nonperturbative MFRTB method to a crystalline silicon immersed in a strong magnetic field. By using the magnetic energy band structure obtained, we show that the second-order phase transition from a band insulator to metal induced by the magnetic field. Therefore, we can say that the crystalline silicon exhibits the second-order phase transition from a band insulator to metal. Thus, we conclude that the magnetization exhibits a kink behavior between 2 $B_c$ (T) and 2 $B_c$ (T). The magnetization that corresponds to first derivative of the total energy with respect to $B$ is continuous across $B_c$, but the second derivative exhibits discontinuity. This suggests that this phenomenon is regarded as the second-order phase transition induced by the magnetic field.

As shown in figure 1, the energy band gap monotonically increases with $B$ up to about $5 \times 10^3$ (T). In magnetic fields above $5 \times 10^3$ (T), the energy band gap shows a decreasing trend with increasing $B$, and eventually reaches zero at $B_c$. This means that the crystalline silicon in strong magnetic fields above $B_c$ changes to metal. Therefore, we can say that the crystalline silicon exhibits the second-order phase transition from a band insulator to metal induced by the magnetic field.

Let us consider this second-order phase transition in more detail by using the magnetic energy band structure obtained in the magnetic BZ. Figure 2 shows $E(k)$ for $B = 743.1$ (T) that is much smaller than $B_c$. The horizontal axes denotes the normalized wavevector $\mathbf{k}$ that is defined as $\mathbf{k} = \frac{2\pi}{a} \mathbf{k}$. In figure 2, $\mathbf{k}$ changes from $R_x$ point ($\mathbf{k} = (1, 0, 0)$) to $\Gamma$ point ($\mathbf{k} = (0, 0, 0)$), and changes from $\Gamma$ point to $R_y$ point ($\mathbf{k} = (1, 0, 0)$) via $\mathbf{k} = (0, 0, 0.5)$. Similar to the MFRTB calculations [33], the nonperturbed MFRTB method also yields nearly flat energy bands in the $k_x - k_y$ plane as shown in figure 2. Nearly flat bands in the $k_x - k_y$ plane imply that the motion of electrons in the plane perpendicular to the magnetic field is essentially changed corresponding to the quantization of the orbital motion of electrons in a magnetic field [33]. The existence of nearly flat bands means that the energy at $(0, 0, \frac{\pi}{a} m)$ is almost same as those at $(0, 0, m\pi)$.
Figure 1. Magnetic-field dependences of the magnetization and energy band gap. The left vertical axis denotes the magnetization that is calculated by the derivative of the total energy with respect to the magnetic field. The right vertical axis denotes the energy band gap of the crystalline silicon immersed in a magnetic field.

Figure 2. The magnetic energy band structure $E(k)$ for $p/q = 1/151$ that corresponds to $B = 743.1(T)$. The $R_x$, $\Gamma$ and $R_z$ points correspond to $k = (1, 0, 0)$, $\Gamma = (0, 0, 0)$ and $k = (0, 0, 1)$, respectively. Magnetic energy bands are nearly flat in the $k_x - k_y$ plane that is perpendicular to the magnetic field.

$(\overline{E}_{3x}, \overline{E}_y, \overline{E}_{3z})$, where $\overline{E}_{3z}$ denotes a certain value of $\overline{E}_z$. This knowledge will be used later in the discussion about the origin of the oscillation of the magnetization.

It is also found from figure 2 that the highest occupied state (HOS) and lowest unoccupied state (LUS) are obtained at $\Gamma$ point and $k = (0, 0, 0.5)$, respectively. The energy band gap at $B = 743.1(T)$ is about 1.504 (eV) \cite{40} that is larger than that for the case of zero magnetic field.

Figures 3(a)–(c) show the magnetic energy bands at (a) $B = 0.99999 \times 10^4$ (T), (b) $B = 1.5554 \times 10^4$ (T) and (c) $B = 2.2156 \times 10^4$ (T), respectively, that are lower than $B_c$. Figure 3(d) shows magnetic energy bands at $B = 2.2220 \times 10^4$ (T) that is higher than $B_c$. The horizontal axes denotes $\overline{k}$ that changes from $\Gamma$ point to $R_x$ point. Comparing figure 3(a) with figure 2, the HOS and LUS still occur at the $\Gamma$ point and near the point of $k = (0, 0, 0.5)$, respectively. Both energy levels of the HOS and LUS decrease with increasing $B$. The characteristic feature in figure 3(a) is that the energy level of the occupied states around the point of $k = (0, 0, 0.5)$ increases with $B$. Comparing figures 3(a) with 3(b), it can be seen that the energy level for the HOS at $\Gamma$ point increases with increasing $B$. As a result, the normalized wavevector that gives the LUS shifts from the $\Gamma$ point to that near the point of $k = (0, 0, 0.5)$ with increasing $B$. In the
Figure 3. Magnetic energy band structures $E(k)$ for (a) $p/q = 9/101$ that corresponds to $B = 9.9991 \times 10^4$ (T), (b) $p/q = 14/101$ that corresponds to $B = 1.5554 \times 10^4$ (T), (c) $p/q = 31/157$ that corresponds to $B = 2.2156 \times 10^4$ (T) and (d) $p/q = 20/101$ that corresponds to $B = 2.2220 \times 10^4$ (T), respectively. The insets in (c) and (d) are magnified views of the magnetic energy band structure near the point of $k = (0, 0, 0.5)$.

As shown in figure 3(d), the energy band gap cannot be found in the magnetic energy band structure for $B = 2.2220 \times 10^4$ (T), i.e., the energy band gap disappears between $2.2156 \times 10^4$ (T) (figure 3(c)) and $B = 2.2220 \times 10^4$ (T) (figure 3(d)). Thus, the disappearance of the energy band gap occurs around the point of $k = (0, 0, 0.5)$ in the magnetic BZ.
Figure 4. Magnetic energy band structures $E(k)$ for (a) $p/q = 13/59$ that corresponds to $B = 2.4725 \times 10^4$ (T), (b) $p/q = 25/113$ that corresponds to $B = 2.4826 \times 10^4$ (T), (c) $p/q = 35/157$ that corresponds to $B = 2.5015 \times 10^4$ (T) and (d) $p/q = 24/107$ that corresponds to $B = 2.5169 \times 10^4$ (T), respectively. The circles indicate the magnetic energy bands mentioned in the text.

As mentioned above, the normalized wavevectors that give the HOS and LUS change with increasing $B$. The reason why the magnetic field dependence of the energy levels differs depending on the wavevector is that the dependence of the orbital hybridization both on the wavevector and on the magnetic field are appropriately taken into account in the non-perturbative MFRTB method [37]. It should be noted that the conventional Hofstadter’s method [28] can hardly explain the magnetic-field induced change in the energy band gap of a crystalline silicon [37].

In the metallic phase ($B > B_c$), the magnetization increases in oscillation with increasing $B$ as shown in figure 1. Since the crystalline silicon is in the metallic phase at strong magnetic fields above $B_c$, the appearance of magnetic oscillation seems to be reasonable. However, it should be notice that there does not exist the Fermi surface for silicon at the zero magnetic field, so that this magnetic oscillation is different from the dHvA oscillation observed in usual metals. The present magnetic oscillations are caused by energy states changing from occupied to unoccupied states with increasing $B$. Indeed, we confirm this description of the magnetic oscillation from the magnetic energy bands obtained in the magnetic BZ. Let us focus on the oscillation peak observed around $B = 2.5 \times 10^4$ (T) in figure 1. Figures 4(a)–(d) show the magnetic energy bands at $B = 2.4725 \times 10^4$ (T), $B = 2.4826 \times 10^4$ (T), $B = 2.5015 \times 10^4$ (T) and $B = 2.5169 \times 10^4$ (T), respectively. As shown in figure 4(a), a set of unoccupied magnetic energy bands exist near $\vec{k} = (0, 0, 0.5)$ in the energy ranging from $-6.57$ (eV) to $-6.55$ (eV). Due to these energy states, the density of states becomes much large. This is because in the plane of $\vec{k}_z = 0.5$ there exist a lot of states.
that have almost the same energy as that with \( \mathbf{k} = (0, 0, 0.5) \) as mentioned above. As shown in figure 4(b), these magnetic energy bands move down with increasing \( B \). These magnetic energy bands move down with increasing \( B \) and eventually become occupied states in figures 4(c) and (d). Corresponding to this change, the magnetization oscillates around \( B = 2.5 \times 10^4 \) (T) as shown in figure 1.

While the magnetization oscillates with increasing \( B \) in magnetic fields above \( B_c \), the magnetization increases without oscillations in magnetic fields below \( B_c \) as shown in figure 1. We shall give a comment on this point. The number of \( \mathbf{k} \)-points in the magnetic BZ is equal to that of the magnetic primitive unit cell contained in the system \([33]\). The number of the magnetic primitive unit cell is given as \( N/q \), where \( N \) denotes the number of the primitive unit cells in the zero magnetic field case \([33, 41]\). Therefore, the number of \( \mathbf{k} \)-points in the magnetic BZ is given by \( N/q \), which means that each magnetic energy band contains \( N/q \) electronic states. Since there are 8\( N \) valence electrons in the system, these electrons will occupy the states of the lower \( 8q \) magnetic energy bands. Even if the magnetic field changes, the lower \( 8q \) magnetic energy bands are occupied until the energy gap disappears. It is shown in the previous work \([34]\) that oscillations in the magnetization such as the dHvA oscillation and additional oscillation peaks \([34]\) occur when magnetic energy bands change from occupied states to unoccupied ones or vice versa. Since the lower \( 8q \) magnetic energy bands are always occupied when an energy gap exists, magnetic energy bands never change from occupied states to unoccupied states or vice versa. Therefore, oscillations in the magnetization would not occur in the band insulator phase.

4. Concluding remarks

In summary, it is found that the second-order phase transition is induced in the crystalline silicon by a strong magnetic field. The critical magnetic field is about \( 2.22 \times 10^4 \) (T). The energy band gap disappears at the critical magnetic field, which means that this transition is recognized as a band insulator to metal transition induced by the magnetic field. It is also found that a magnetic oscillation in the magnetization appears after the transition. This is because the magnetic energy bands in the magnetic BZ change from the occupied to unoccupied states or vice versa.

We shall give a brief comment on the magnitude of the critical magnetic field. In this work, we have treated the second-order phase transition of the crystalline silicon that has an energy band gap of about 1.1 (eV) at zero magnetic field. For materials with smaller energy band gaps than silicon, such as InSb and InAs, it is expected that the energy band gap disappears at smaller magnetic fields. Namely, the critical magnetic field is expected to be smaller than \( 2.22 \times 10^4 \) (T) for materials with smaller energy band gaps. Calculations for such materials will be the subject of future work.

The effect of the electron–electron interaction is not considered in the present calculations. For more accurate description of the second-order phase transition, the effect of electron–electron interaction should be taken into account. For example, the current–density functional theory can be used for this aim \([42–45]\). It seems to be interesting to investigate how the electron–electron interaction changes the magnetic energy band structure of silicon immersed in a magnetic field and to what extend it makes revisions to the second-order phase transition phenomena in the present case.

Acknowledgments

This work was partially supported by Grant-in-Aid for Scientific Research (Nos. 18K03510 and 18K03461) of the Japan Society for the Promotion of Science.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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