

**Mechanism of Fermi level pinning at metal/germanium interfaces**K. Kasahara,<sup>1</sup> S. Yamada,<sup>1</sup> K. Sawano,<sup>2</sup> M. Miyao,<sup>1</sup> and K. Hamaya<sup>1,3,\*</sup><sup>1</sup>*Department of Electronics, Kyushu University, 744 Motoooka, Fukuoka 819-0395, Japan*<sup>2</sup>*Advanced Research Laboratories, Tokyo City University, 8-15-1 Todoroki, Tokyo 158-0082, Japan*<sup>3</sup>*PRESTO, Japan Science and Technology Agency, Sanbancho, Tokyo 102-0075, Japan*

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The physical origin of Fermi level pinning (FLP) at metal/Ge interfaces has been argued over a long period. Using the Fe<sub>3</sub>Si/Ge(111) heterostructure developed originally, we can explore electrical transport properties through atomically matched metal/Ge junctions. Unlike the conventional metal/*p*-Ge junctions reported so far, we clearly observe rectifying current-voltage characteristics with a measurable Schottky barrier height, depending on the contact area of the Fe<sub>3</sub>Si/Ge(111) junction. These results indicate that one should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces. This study will be developed for understanding FLP for almost all the metal/semiconductor interfaces.

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**I. INTRODUCTION**

The fundamental mechanism of the formation of the Schottky barrier at metal/semiconductor interfaces has so far been studied over a long period.<sup>1-9</sup> In particular, the controversy about the physical origin of Fermi level pinning (FLP) at the metal/semiconductor interfaces remains unsolved.<sup>10</sup> In order to interpret FLP, the metal-induced gap states (MIGSs),<sup>1,6</sup> caused by the decay of the traveling-wave function from the metal electrode into the band gap of the semiconductor, have been suggested. The MIGSs are considered to be intrinsic mechanisms. In contrast, other extrinsic mechanisms such as defect-induced gap states at the interface have been discussed.<sup>3,5,8</sup>

Development of high mobility germanium (Ge)-based metal-oxide-semiconductor field effect transistors (MOSFETs) is required for breaking down the ultimate scaling limit of silicon (Si)-based conventional complementary metal-oxide-semiconductor transistors.<sup>11</sup> However, FLP is one of the critical issues even at metal/Ge interfaces,<sup>10</sup> disturbing the development of high-performance MOSFETs with metallic source and drain contacts. In general, the influence of FLP on metal/Ge interfaces is stronger than that on metal/Si ones. The strong FLP always results in relatively high Schottky barrier height (SBH:  $\Phi_b \sim 0.6$  eV) for metal/*n*-Ge junctions and Ohmic characteristics for metal/*p*-Ge ones, arising from the charge neutrality level close to the valence-band edge of Ge.<sup>12,13</sup>

Recently, effective alleviation of the strong FLP was also demonstrated by an insertion of ultrathin insulating layers between a metal and Ge,<sup>14,15</sup> in which electrical properties of the metal/*n*-Ge and metal/*p*-Ge junctions were varied to Ohmic and rectifying characteristics with increasing the thickness of the insertion layer. It seems that the observed thickness dependence is strongly related to the blocking of the penetration of the wave function of electrons in the band gap of Ge. Thus one has believed that the strong FLP at metal/Ge interfaces is predominantly due to MIGSs,<sup>14-16</sup> i.e., intrinsic mechanisms. On the other hand, several groups have discussed the influence of extrinsic mechanisms such as dangling bonds on the strong FLP.<sup>17-21</sup> Therefore exploring the mechanism of FLP at metal/Ge interfaces is not only important

for demonstrating high-performance MOSFETs but also for understanding FLP for almost all the metal/semiconductor interfaces.

In order to elucidate the origin of the strong FLP, we propose that the use of the high-quality Fe<sub>3</sub>Si(111)/Ge(111) junction with an atomically matched interface is effective.<sup>20</sup> Fe<sub>3</sub>Si has a Heusler-type crystal structure<sup>22,23</sup> and there is almost no lattice mismatch between Fe<sub>3</sub>Si (0.564–0.566 nm) and Ge (0.565 nm). Furthermore, the atomic matching at the junction between Fe<sub>3</sub>Si(111) and Ge(111) is theoretically perfect, as illustrated in Fig. 1 of Ref. 20. To date, we clarified that, for Fe<sub>3</sub>Si/*n*-Ge(111) junctions, the SBH is unexpectedly lower ( $\Phi_b \sim 0.46$  eV) than that due to the strong FLP reported so far (0.55–0.65 eV) and, for Fe<sub>3</sub>Si/*p*-Ge(111) junctions, rectifying behavior in current-voltage (*I*-*V*) characteristics is seen below 170 K.<sup>20</sup> Though these results have implied the presence of an extrinsic mechanism of the strong FLP, we have not yet obtained its reliable evidence. At least, we should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces.

In this paper, we experimentally study the mechanism of the strong FLP at metal/Ge interfaces using the atomically matched Fe<sub>3</sub>Si/Ge(111) heterostructure. For the high-quality Fe<sub>3</sub>Si/*p*-Ge(111) junctions, we can easily observe the clear Schottky characteristics with a measurable Schottky barrier height, depending on the contact area of the Fe<sub>3</sub>Si/Ge(111) junction. These transport data can be understood by the model based on the influence of the interfacial defects such as dangling bonds, and indicate that one should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces. This study will be developed for understanding FLP for almost all the metal/semiconductor interfaces.

**II. SAMPLES AND MEASUREMENTS**

Prior to the fabrication of the Fe<sub>3</sub>Si/Ge(111) heterostructure, *p*-Ge(111) substrates were chemically cleaned to remove contamination and native oxide from the surface, where the *p*-Ge(111) substrates were already on the market ( $p = 9 \times 10^{14}$  cm<sup>-3</sup>). The cleaned substrates were loaded immediately

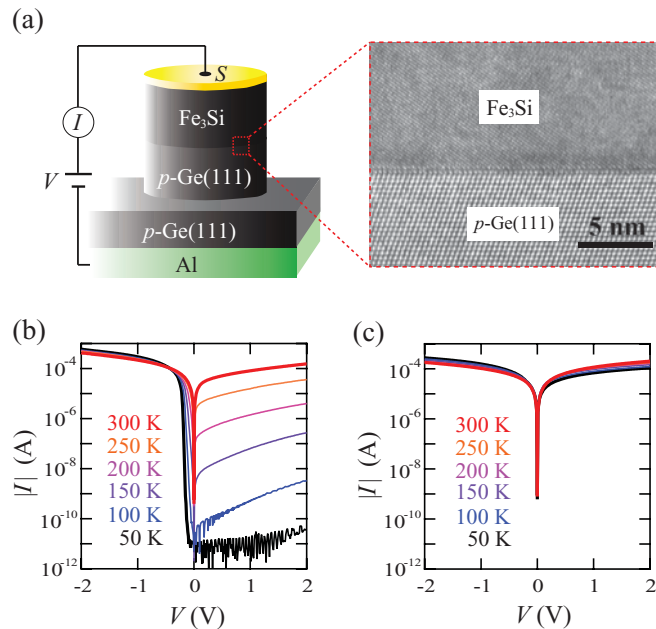


FIG. 1. (Color online) (a) The schematic illustration of the fabricated junctions with various areas ( $S$ ). The enlarged picture is a cross-sectional transmission electron micrograph of the atomically controlled Fe<sub>3</sub>Si/Ge(111) interface. (b),(c)  $I$ - $V$  characteristics of representative two junctions with  $S \sim 1 \mu\text{m}^2$ . (b) Marked rectifying and (c) Ohmic behavior with the temperature evolution.

into an ultrahigh vacuum chamber with a base pressure of  $\sim 10^{-7}$  Pa. After the surface heat treatment conducted at  $550^\circ\text{C}$  for 20 min, the substrate temperature was reduced down to  $200^\circ\text{C}$ . An atomically clean surface was confirmed by observing the reflection high-energy electron diffraction (RHEED) patterns. Using low-temperature molecular-beam epitaxy (MBE),<sup>24</sup> we grew the epitaxial Fe<sub>3</sub>Si layer with a thickness of 50 nm on  $p$ -Ge(111). During the growth, two-dimensional epitaxial growth was confirmed by the observation of RHEED patterns. After the growth, we fabricated Schottky diodes with a contact area  $S$  ( $S \sim 1$ ,  $\sim 10^2$ ,  $\sim 10^4$ , and  $\sim 10^6 \mu\text{m}^2$ ) to examine electrical properties of the Fe<sub>3</sub>Si/ $p$ -Ge(111) junctions.<sup>20</sup> Here all the diodes used in this study were fabricated from one Fe<sub>3</sub>Si/ $p$ -Ge(111) wafer. The schematic diagram of the fabricated Fe<sub>3</sub>Si/ $p$ -Ge(111)/Al Schottky junctions is shown in Fig. 1(a), where a backside Al is an Ohmic contact. The Fe<sub>3</sub>Si/Ge(111) interface is atomically flat,<sup>20,24</sup> as shown in a cross-sectional transmission electron micrograph (TEM) image in Fig. 1(a). To compare the atomically matched high-quality junctions with other mismatched ones, we also fabricated Al/ $p$ -Ge(111) junctions with the atomically mismatched interface by using the same MBE equipment after the same surface cleaning. The growth temperature of the Al/ $p$ -Ge(111) junctions was less than  $25^\circ\text{C}$ .

### III. RESULTS AND DISCUSSION

We have studied  $I$ - $V$  characteristics for lots of Fe<sub>3</sub>Si/ $p$ -Ge(111) junctions with  $S \sim 1 \mu\text{m}^2$ . Figures 1(b) and 1(c) show representative  $I$ - $V$  characteristics at various temperatures. Despite the directly connected metal/Ge structure, we observe marked rectifying behavior in Fig. 1(b) at low

temperatures surprisingly. The ratio of the forward current ( $I_{\text{ON}}$ ) to the reverse current ( $I_{\text{OFF}}$ ) reaches  $\sim 10^8$  at 50 K. The reverse bias current ( $V > 0$ ) increases with increasing temperature, implying the presence of an evident Schottky barrier. A rectifying  $I$ - $V$  characteristic can be obtained even at 300 K. Using the thermionic emission theory,<sup>25</sup> we can roughly obtain  $\Phi_b$  for hole transport. From the  $I$ - $T$  characteristics,<sup>20</sup> the  $\Phi_b$  for holes in Fig. 1(b) was estimated to be  $\sim 0.18$  eV, which is the first experimental observation of  $\Phi_b$  in the directly connected metal/ $p$ -Ge junctions. In contrast, almost Ohmic characteristics are seen in Fig. 1(c) even at low temperatures, consistent with the strong FLP.<sup>12,13</sup> This means that the tunneling conduction occurs through the very low and thin Schottky barrier. When we decreased temperature from 50 to 10 K, we observed very small rectifications in  $I$ - $V$  characteristics (not shown here). Note that despite almost the same devices fabricated from the same wafer there are different  $I$ - $V$  characteristics for Fe<sub>3</sub>Si/ $p$ -Ge(111) junctions with  $S \sim 1 \mu\text{m}^2$ . We also measured the  $I$ - $V$  characteristics of the Al/ $p$ -Ge(111) junctions with  $S \sim 1 \mu\text{m}^2$ , measured at various temperatures, and then, almost all the junctions showed Ohmic  $I$ - $V$  characteristics, also consistent with the strong FLP.<sup>12,13</sup> For the Al/ $p$ -Ge(111) junctions, we sometimes observed very small rectifications in  $I$ - $V$  characteristics as the temperature was decreased down to 10 K. However, we could not estimate  $\Phi_b$  for Al/ $p$ -Ge(111). We emphasize that clear Schottky characteristics were achieved only when we used the atomically matched Fe<sub>3</sub>Si/Ge(111) interface.

To understand the interesting features described above, we further examined the effect of  $S$  on  $I$ - $V$  characteristics for many junctions in detail. As a consequence, we easily observed rectifying behavior in the  $I$ - $V$  curves at low temperatures for many Fe<sub>3</sub>Si/ $p$ -Ge(111) junctions. In Fig. 2 we summarize  $I_{\text{ON}}/I_{\text{OFF}}$  at 100 K for various Fe<sub>3</sub>Si/ $p$ -Ge(111) junctions with  $S \sim 1$ ,  $\sim 10^2$ , and  $\sim 10^4$ – $10^6 \mu\text{m}^2$ , together with the data for

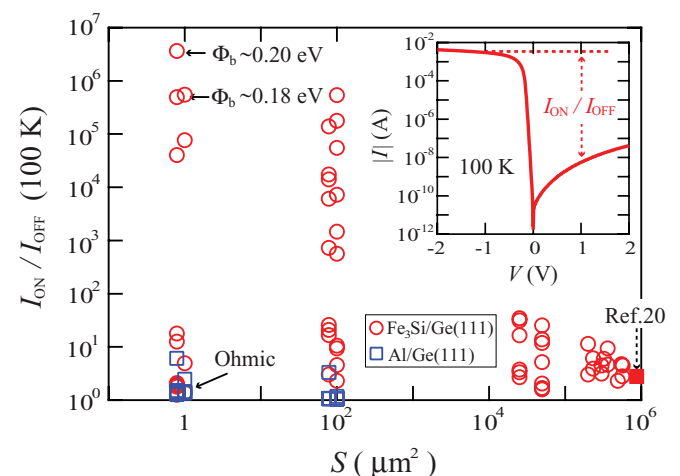


FIG. 2. (Color online) Summary of  $I_{\text{ON}}/I_{\text{OFF}}$  ratio measured at 100 K for various Fe<sub>3</sub>Si/ $p$ -Ge(111)/Al junctions (red) with  $S \sim 1$ ,  $\sim 10^2$ , and  $\sim 10^4$ – $10^6 \mu\text{m}^2$ , together with that for Al/ $p$ -Ge(111)/Al (blue) junctions. The red-square symbol at  $\sim 10^6 \mu\text{m}^2$  is the data for a sample shown in Ref. 20. The inset shows an  $I$ - $V$  characteristic for a junction with  $S \sim 10^2 \mu\text{m}^2$  at 100 K. The  $I_{\text{ON}}/I_{\text{OFF}}$  ratio is defined at  $V = \pm 1$  V.

Al/*p*-Ge(111) junctions. Here for all kinds of  $S$  we measured  $I$ - $V$  curves of more than 15 junctions, and the  $I_{ON}/I_{OFF}$  values were roughly defined as the data at  $V = \pm 1$  V, as shown in the inset. In the main figure we can reconfirm that, for the Al/*p*-Ge(111) junctions with the atomically mismatched interfaces, all the  $I_{ON}/I_{OFF}$  values are less than  $10^1$  even for the smallest junctions with  $S = \sim 1 \mu\text{m}^2$ , consistent with the strong FLP. On the other hand, for the  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  junctions, we can evidently see the difference in the  $I_{ON}/I_{OFF}$  values depending strongly on  $S$ . For the large junctions ( $S = \sim 10^6 \mu\text{m}^2$ ), the  $I_{ON}/I_{OFF}$  values are almost constant ( $\sim 10^1$ ). The small rectification of the  $I$ - $V$  curves disappeared at  $\sim 170$  K, similar to our previous work.<sup>20</sup> In contrast, for the small junctions with  $S = \sim 1$  and  $\sim 10^2 \mu\text{m}^2$ , the  $I_{ON}/I_{OFF}$  values are scattered from the wide range  $10^0 \leq I_{ON}/I_{OFF} \leq 10^7$ . For  $S = \sim 1 \mu\text{m}^2$  the junctions shown in Figs. 1(b) and 1(c), i.e.,  $\Phi_b \sim 0.18$  eV and Ohmic, respectively, are also plotted in Fig. 2 (see arrows), and the junction with  $\Phi_b \sim 0.20$  eV shows the largest  $I_{ON}/I_{OFF} \sim 7 \times 10^6$ . The scattering of the  $I_{ON}/I_{OFF}$  values in Fig. 2 implies that many kinds of the Schottky barriers are distributed for our  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  junctions. We discuss it later. Note that the scattering range for  $S = \sim 1 \mu\text{m}^2$  is narrow ( $I_{ON}/I_{OFF} < \sim 10^1$ ,  $\sim 10^5 < I_{ON}/I_{OFF} < 10^7$ ) compared to  $S = \sim 10^2 \mu\text{m}^2$  ( $I_{ON}/I_{OFF} < \sim 10^2$ ,  $10^3 < I_{ON}/I_{OFF} < 10^6$ ).

Hereafter we intensively discuss the effect of  $S$  on  $I_{ON}/I_{OFF}$ , presented in Fig. 2. For almost all the Al/*p*-Ge(111) junctions, we can regard the small  $I_{ON}/I_{OFF}$  values of  $\sim 10^0$  at low temperatures as consequences of the strong influence of FLP on the hole transport. In short, there is almost no effect of  $S$  on  $I_{ON}/I_{OFF}$  at low temperatures. On the other hand, there is a marked effect of  $S$  on  $I_{ON}/I_{OFF}$  for the  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  junctions. Even if we use the atomically matched  $\text{Fe}_3\text{Si}(111)/\text{Ge}(111)$  junctions shown in Fig. 1 of Ref. 20, there will be still some atomic imperfection at the (111) planes between Fe or Si in  $\text{Fe}_3\text{Si}$  and Ge, giving rise to the defects such as dangling bonds in Ge at the interface. Therefore the presence of some unintentional defects at the  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  interface can be considered generally. In general, since the number of defects can be expressed by assuming Poisson distribution, we can show a possible scenario considering the correlation between  $S$  and interfacial defects as follows. When  $S$  is large such as  $S = \sim 10^6 \mu\text{m}^2$ , the  $\text{Fe}_3\text{Si}/\text{Ge}(111)$  junction includes the some interfacial defects, as schematically illustrated in Fig. 3(a). The observed small  $I_{ON}/I_{OFF}$  values of  $\sim 10^1$  in Fig. 2 should be regarded as consequences of the influence of the interfacial defects on hole transport properties. On the other hand, when we reduce  $S$  as small as possible, we can encounter the two different interfaces, as shown in Fig. 3(b). Then, we can obtain almost no or a strong contribution of the defects to the transport properties. Surely, for  $S = \sim 1 \mu\text{m}^2$ , we have already obtained such two different contributions in Figs. 1(b) and 1(c). Also, we can regard the two discrete regions in Fig. 2, i.e.,  $I_{ON}/I_{OFF} < \sim 10^1$  and  $\sim 10^5 < I_{ON}/I_{OFF} < 10^7$ , as the above two different contributions. In contrast, since there are a large number of interfacial defects at the atomically mismatched Al/*p*-Ge(111) interfaces, as illustrated in Fig. 3(c), we cannot encounter the situation with almost no interfacial defect even if we use the small junctions that we can fabricate. Since we have not obtained the data with Schottky characteristics even for the smallest Al/*p*-Ge(111) junctions, the above scenario

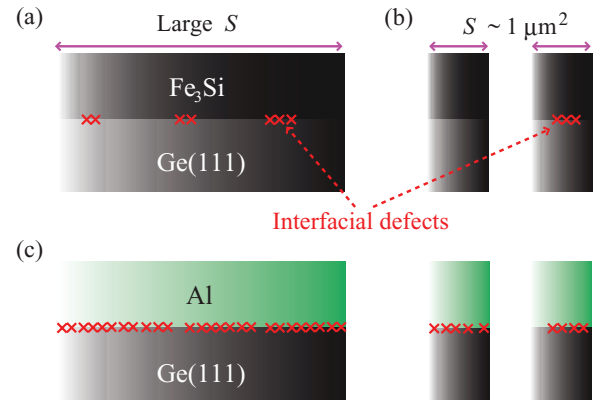


FIG. 3. (Color online) The schematic diagrams of the model for the  $\text{Fe}_3\text{Si}/\text{Ge}(111)$  interface with (a) large  $S$  and (b) small  $S$ . There are some interfacial defects even at the atomically matched interface. (c) The diagrams in the case of the atomically mismatched Al/*p*-Ge(111) interface.

based on the influence of the interfacial defects on the hole transport can also be applied to the atomically mismatched interfaces.

Recent papers also indicated that passivation techniques of the Ge surface can work effectively for changing electrical properties of the metal/Ge junctions.<sup>18,19,21</sup> Also, theoretical studies suggested that the defect levels lie just above the valence band,<sup>26,27</sup> indicating that the previous experimental results shown in Refs. 12 and 13 originate from the interfacial defects such as dangling bonds. These studies strongly support our new findings in this paper. We want to emphasize that lots of researchers have so far observed the predominant influence of interfacial defects on the transport properties of metal/Ge junctions. In other words, this study indicates that if one discusses the fundamental mechanism of the formation of the Schottky barrier at metal/Ge interfaces, one should consider the influence of interfacial defects, i.e., extrinsic mechanisms. In the future, we will need further exploration of the method for reducing the number of the defects formed at the atomically matched metal/Ge interfaces.

Finally, we discuss the scattering of the  $I_{ON}/I_{OFF}$  values in Fig. 2 for  $S = \sim 1$  and  $\sim 10^2 \mu\text{m}^2$ . For  $S = \sim 1 \mu\text{m}^2$ , the various  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  interfaces with Schottky barriers from  $\Phi_b \sim 0.20$  eV to almost Ohmic were demonstrated. Also, the scattering range for  $S = \sim 1 \mu\text{m}^2$  is narrower than that for  $S = \sim 10^2 \mu\text{m}^2$ . This feature indicates that the scattering of the  $I_{ON}/I_{OFF}$  values is related to  $S$ , i.e., the number of interfacial defects. Since the  $I_{ON}/I_{OFF}$  value is usually attributed to  $\Phi_b$ , we should interpret that  $\Phi_b$  is also related to the number of defects. Thus somewhat different contributions of the number of defects to  $\Phi_b$  can be considered in the  $\text{Fe}_3\text{Si}/\text{Ge}(111)$  junctions. On the basis of this consideration, we show interesting findings for electrical properties in the  $\text{Fe}_3\text{Si}/\text{Ge}(111)$  junctions. Figure 4(a) displays the  $I$ - $V$  curves for an  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  junction with  $S = \sim 10^2 \mu\text{m}^2$  at various temperatures. Interestingly, we can see the staircaselike  $I$ - $V$  characteristics in forward bias ( $V < 0$ ), denoted by I, II, and III. In this study, we frequently observed these staircaselike  $I$ - $V$  characteristics for  $S = \sim 10^2 \mu\text{m}^2$  at low temperatures though the room-temperature  $I$ - $V$  curves



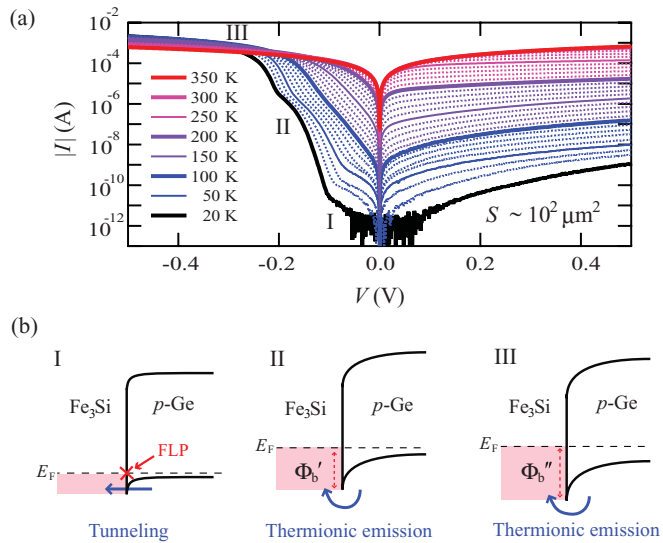


FIG. 4. (Color online) (a) Temperature evolution of  $I$ - $V$  characteristics with three-step staircase in forward bias ( $V < 0$ ), observed in  $\text{Fe}_3\text{Si}/\text{Ge}(111)$  junctions with  $S = \sim 10^2 \mu\text{m}^2$ . (b) Schematic illustrations of the hole transport in  $V < 0$  at low temperatures. There are plural current channels in the  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  junctions and all the channels contribute to the forward-bias current.

were almost the same Ohmic characteristics. The interpretation of the staircaselike  $I$ - $V$  characteristics is shown in Fig. 4(b). That is, there are plural current channels for holes, resulting from the tunneling conduction due to FLP (I) and from the thermionic-emission conduction (II, III) with two different Schottky barriers with  $\Phi_b'$  and  $\Phi_b''$ . At low temperatures the forward bias current ( $V < 0$ ) can detect the contributions of all the current channels, while, with increasing temperature,  $\Phi_b'$  and  $\Phi_b''$  cannot affect the transport properties, giving rise to the

disappearance of the staircaselike behavior. This feature means that there are different contributions of the interfacial defects to  $\Phi_b$  for just one  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  interface in the middle-sized junctions. By using the atomically matched  $\text{Fe}_3\text{Si}/p\text{-Ge}(111)$  interface, we can evidently observe some different findings for electrical properties of metal/Ge interfaces. This study indicates that one should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces.

#### IV. CONCLUSION

We have studied the mechanism of FLP at metal/Ge junctions using the atomically matched  $\text{Fe}_3\text{Si}/\text{Ge}(111)$  interface. Despite metal/ $p$ -Ge interfaces, we clearly observed rectifying current-voltage characteristics with a measurable Schottky barrier height, depending on the contact area of the  $\text{Fe}_3\text{Si}/\text{Ge}(111)$  junction. These data can be understood by the model based on the influence of the interfacial defects such as dangling bonds, and indicate that one should distinguish between intrinsic and extrinsic mechanisms for discussing the formation of the Schottky barrier at metal/Ge interfaces. This study will give us an important principle for understanding FLP for almost all the metal/semiconductor interfaces, which has been studied over a long period.

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\*hamaya@ed.kyushu-u.ac.jp

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