BNL-111930-2016-JA

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In-implanted Ge by C co-doping***

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Submitted to the Journal of Applied Physics Letters

November 2015

**Nuclear Science & Technology Department
Brookhaven National Laboratory**

U.S. Department of Energy

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Enhanced electrical activation in In-implanted Ge by C co-doping

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(Received 10 September 2015; accepted 11 November 2015)

At high dopant concentrations in Ge, electrically activating all implanted dopants is a major obstacle in the fulfillment of high-performance Ge-channel complementary metal oxide semiconductor devices. In this letter, we demonstrate a significant increase in the electrically-active dopant fraction in In-implanted Ge by co-doping with the isovalent element C. Electrical measurements have been correlated with x-ray absorption spectroscopy and transmission electron microscopy results in addition to density functional theory simulations. With C + In co-doping, the electrically active fraction was doubled and tripled at In concentrations of 0.2 and 0.7 at. %, respectively. This marked improvement was the result of C-In pair formation such that In-induced strain in the Ge lattice was reduced while the precipitation of In and the formation of In-V clusters were both suppressed. [<http://dx.doi.org/10.1063/1.4936331>]

Source and drain regions in complementary metal oxide semiconductor (CMOS) devices necessitate high dopant concentrations to reduce contact resistance and improve device performance.¹ Attaining a sufficient electrically-active dopant fraction is a substantial challenge at high dopant concentrations. In the first instance, the maximum electrically-active dopant fraction is limited by the solid solubility. As this threshold is approached, the formation of electrically-inactive dopant-atom clusters (D_n) and/or dopant-vacancy complexes (D_nV_m) is triggered.²⁻⁶ When the threshold is exceeded, dopants may also precipitate.

While Ge is considered a promising candidate to replace Si in future high-mobility CMOS devices,^{7,8} the low solid solubility of dopants in Ge is a major obstacle.⁹ In has attracted recent interest as a potential *p*-type dopant in Ge due to a low activation energy of 0.0112 eV.¹⁰⁻¹² In a previous study of In-implanted Ge, we reported a decrease in the electrically-active dopant fraction for In concentrations >0.2 at. % as a result of the formation of electrically-inactive In metal precipitates and In-V clusters¹³ as consistent with earlier density functional theory (DFT) calculations.^{14,15} The solid solubility of In in Ge was found to be between 0.2 and 0.6 at. % at maximum annealing temperature of 550 °C,¹³ yet the source and drain regions in future CMOS device required dopant concentration above 1 at. %.¹ To meet a more aggressive electrical activation target at advanced device dimensions, an above-equilibrium, metastable solid solubility limit for In in Ge is required.¹ To this end, several methods to enhance the electrically-active dopant fraction have been considered: rapid thermal annealing,¹⁶ excimer laser annealing,¹⁷ and flash annealing¹⁸ have all been successfully utilized to achieve an electrically-active B concentration in Ge in excess of the solid

solubility limit as has pre-amorphization followed by solid phase epitaxy.^{9,19} An important alternative is co-doping including double donor doping²⁰ and F co-doping,²¹ both of which were beneficial for *n*-type dopant activation in Ge. Chrones²² recently reviewed co-doping strategies for Ge, concluding that co-doping (with double donors, F or isovalent atoms) is advantageous for controlling the vacancy (V) concentration. As above, this point defect is a key component of the electrically-inactive dopant cluster D_nV_m .

As an isovalent element to Ge, C is a promising option for co-doping with In. C + In co-doping in Si has been previously studied with both experiment and simulation: Rutherford backscattering spectroscopy (RBS),²³ spreading resistance profiling,²⁴ x-ray absorption spectroscopy (XAS),^{25,26} and DFT calculations^{27,28} demonstrated that C and In atoms have a preference for pairing such that In precipitation was suppressed and high electrically-active dopant fractions were achieved. Intuitively, a similar effect can be anticipated in Ge. Supporting evidence includes perturbed angular correlation (PAC)²⁹ measurements that indicated 34% of In probes paired with C atoms on substitutional sites after 600 °C annealing (as attributed to strain compensation between undersized C atoms and oversized In atoms²⁹) and recent DFT calculations that C-In pair formation in Ge was energetically favorable (with a binding energy of -0.46 eV).³⁰ In this report, we correlate electrical and structural measurements in C + In co-doped Ge to not only demonstrate C-In pairing but also to identify the mechanisms by which a three-fold enhancement of electrically-active dopant fraction has been attained. We also examine a range of C and In concentrations, the latter at device-appropriate levels, to establish the concentration-dependent effectiveness of this approach.

Undoped Ge layers of thickness 1.8 μm , deposited on (100) Si substrates by ultra-high vacuum chemical vapor

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deposition, were implanted with C and In ions. We used a Ge/Si heterostructure to enable the subsequent removal of the Si substrate for superior synchrotron-based measurements.¹³ The influence of misfit dislocations near the Ge/Si interface (due to the lattice mismatch between Ge and Si) was minimized by confining the implanted C and In depth distributions to $<1.2\ \mu\text{m}$. Implantations were performed at $250\ ^\circ\text{C}$ to avoid amorphization and the surface normal was offset 7° from the incident ion direction to avoid channeling. C ions were first implanted, with four ion energies (100, 200, 450, and $750\ \text{keV}$) and variable fluences (7.73×10^{14} – 3.74×10^{16} ions/ cm^2) to produce a uniform C depth distribution over 0.2 – $1.2\ \mu\text{m}$, as calculated with TRIM-2008.³¹ In ions were then implanted with ion energies and fluences appropriate to yield overlapping C and In depth distributions, and at the same concentration to C in each sample (C: In = 1:1). The In implantation details are given in a previous report.¹³ The In concentrations (0.07–1.3 at. %) were determined with RBS after annealing. A three-step annealing process in N_2 , at temperatures of 550, 450, and $350\ ^\circ\text{C}$ for 0.5, 1, and 2 h, respectively, was used to initially activate the implanted In atoms and reduce lattice disorder ($550\ ^\circ\text{C}$) and then enhance the concentration of In-defect configuration by lowering the solid solubility limit ($350\ ^\circ\text{C}$). For the electrical characterization, samples were patterned into clover-leaf van der Pauw geometries of 1 cm radius for high measurement accuracy³² by means of photolithography and H_2O_2 etching at room temperature. To achieve an Ohmic contact, four $0.75\ \text{mm}$ diameter, $200\ \text{nm}$ thick Al contacts were thermally evaporated on the corners of the sample surface. The Ohmic nature of the contacts was confirmed with I-V measurements. Fluorescence-mode extended x-ray absorption fine structure (EXAFS) measurements were performed at the XAS beamline of the Australian Synchrotron, with data analysis carried out using the IFFEFIT package³³ and FEFF9 code.³⁴ Complimentary DFT simulations were performed using the VASP code.³⁵ DFT guided EXAFS analysis was performed, and the input models to the EXAFS spectrum fittings were geometrically-optimized by DFT, a previous applied strategy.^{36–38} The fitting parameters, including In metal fraction, coordination number (CN), and Debye-Waller factors (DWFs), are given

in Table I. Cross-sectional transmission electron microscopy (TEM) images were acquired in a Phillips CM300 electron microscope operating at $300\ \text{kV}$. Samples were prepared with conventional methods of mechanical grinding and polish using Ar ion milling, with the sample maintained at liquid N_2 temperature.

Figure 1 compares the resistivity, carrier density, and carrier mobility of In and C + In implanted Ge samples as a function of In concentration. All samples exhibited *p*-type conductivity. At low In concentrations (~ 0.06 at. %), the effect of co-doping was negligible with the vast majority of In atoms electrically active either with or without C present. Indeed, analysis of the XAS spectra of Figure 2 indicated that In atoms occupied substitutional lattice sites and were four-fold coordinated with or without C present, thus corroborating the electrical measurements. (CNs surrounding an In atom are shown in Table I.) Clearly, the low concentration (~ 0.06 at. %) of both C and In atoms yielded a low probability for C-In pair formation. Also, no evidence of electrically-inactive configurations (In metal precipitates or In-V clusters as shown in Table I) was apparent with XAS at this concentration (~ 0.06 at. %). Finally, the TEM images of Figures 3(a) and 3(d), In and C + In co-doped samples, respectively, show no significant differences in structural disorder.

As Figure 1 demonstrates, the influence of co-doping was more significant at higher In concentrations. At 0.2 at. %, the carrier density of the C + In implanted sample doubled from the In implanted sample (activation ratio increased from 42.3% to 85.9%). While the carrier mobility decreased (by 30%) as a result of increased lattice disorder and ionized impurity scattering, the resistivity was halved in the co-doped sample. Evidence of C-In pairing was found in the DFT-guided EXAFS analysis of this sample (0.2 at. %). The DFT calculations showed that a substitutional C-In pair in Ge splits the Ge second and third shells surrounding an In atom into six different shells (with distances of 3.51, 4.10, 4.38, 4.45, 4.82, and $5.09\ \text{\AA}$). This increase of disorder surrounding an In atom was manifested as smearing of the second and third nearest neighbor peaks of the corresponding FT EXAFS spectrum (Figure 2(d)). Using the DFT-geometrically-optimized model of an C-In pair in substitutional sites of Ge, a high quality fit to the EXAFS spectrum

TABLE I. The In metal fraction, coordination numbers of the first nearest neighbor Ge and C to In, (CN_{Ge} and CN_{C} , respectively) and Debye-Waller factors (DWFs) of the first, second, and third Ge shells, respectively, of the In doped Ge and C + In doped Ge samples. Reproduced with permission from J. Appl. Phys. **118**, 165701 (2015). Copyright 2015 AIP Publishing LLC.

In (and C) concentration (at. %)	In metal fraction (%)	CN_{Ge} (atoms)	CN_{C} (atoms)	DWFs ($\times 10^{-3}\ \text{\AA}^2$)
In doped Ge ^a				
0.02	0	4	$\sim$	3.2, 4.1, 6.4
0.06	0	4	$\sim$	3.4, 4.6, 7.1
0.2	0	4	$\sim$	3.6, 5.1, 7.4
0.6	63 ± 4	3.1 ± 0.4	$\sim$	3.6, 5.5, 7.1
1.2	72 ± 5	2.6 ± 0.5	$\sim$	3.9, 5.6, 6.8
C + In doped Ge				
0.07	0	4	0	3.3, 4.2, 6.7
0.2	0	3.65 ± 0.17	0.35 ± 0.17	3.5, 4.9, 7.3
0.65	0	3.45 ± 0.11	0.55 ± 0.11	3.8, 5.5, 7.7
1.3	0	2.71 ± 0.11	1.29 ± 0.11	4.2, 6.3, 9.4

^aReference 13.

FIG. 1. (a) Resistivity, (b) carrier density, and (c) carrier mobility as a function of In concentration. Squares and circles represent In-doped Ge and C + In co-doped Ge, respectively. In panel (b), unbracketed and bracketed numbers are the electrically-active fractions for In-doped Ge and C + In co-doped Ge, respectively. Reproduced with permission from J. Appl. Phys. **118**, 165701 (2015). Copyright 2015 AIP Publishing LLC.

was obtained for this sample (0.2 at. %) (Figure 2(d)). Note not all In atoms were paired: on average, one In atom was coupled to 0.35 ± 0.07 C atoms as shown in Table I, a result in agreement with earlier PAC measurements.²⁹ Our DFT calculations also supported the result by showing that C-In pairing is energetically favorable in Ge, the binding energy of the cluster is -0.27 eV, in agreement with the previous DFT study (-0.46 eV).³⁰ At this concentration (0.2 at. %), we attribute the enhanced carrier density in the C + In implanted sample to strain compensation by C-In pairing and not the suppression of In precipitation or In-V cluster formation. This was further validated by (i) Raman Spectroscopy (not shown), which indicated that strain in the Ge lattice was reduced with C co-doping and (ii) the XAS results for In-doped Ge without C where the two electrically-inactive configurations were not apparent (Figures 2(a) and 2(c)). Regarding (ii), the defect concentrations were expected to be lower than the sensitivity limit of EXAFS ($\sim 15\%$).

The greatest effect of C + In co-doping was observed at an In concentration of 0.6 at. %. Without C, the electrically-active dopant fraction was only 21% (Figure 1) as a result of the formation of electrically-inactive configurations.¹³ For example, the corresponding XAS spectra (Figures 2(a) and 2(c)) was dominated by a metallic In component (apparent upon comparison with the In metal standard), with $63\% \pm 4\%$ (Table I) of In atoms in the metallic phase. Those In atoms still in solution (the peak at a non-phase-corrected radial distance of ~ 2 Å) were on average surrounded by 0.9 ± 0.4 vacancy (an In-V cluster) and 3.1 ± 0.4 Ge atoms as shown in Table I. Metallic In precipitates were evident in the corresponding TEM image (Figure 3(b)) while line defects (dislocations) were observable in the associated dark-field image (inset). At the similar concentration (0.65 at. %), C + In co-doping yielded a three-fold improvement in electrically-active fraction ($\sim 63\%$, from Figure 1). The corresponding XAS spectra (Figures 2(b) and 2(d)) remain similar to that of substitutional, four-fold coordinated In with no evidence of metallic In or In-V clusters, a result consistent with the co-doping strategies proposed by Chronos²² that the V concentration can be controlled by isovalent element co-doping in Ge. Applying the same EXAFS analysis method aforementioned to the spectrum of this sample (0.65 at. % C + In doped Ge), we found that one In atom was on average paired with 0.55 ± 0.11 C atoms (Table I). Note that no In precipitates were observed in the TEM image of Figure 3(e), demonstrating the effectiveness of co-doping as a means of achieving an above-equilibrium solid solubility limit. For this sample (0.65 at. % C + In doped Ge), the three-fold enhancement of the electrically-active dopant fraction is mainly a result of C co-doping in suppression of the formation of In metal and In-V cluster.

At the highest In concentration of 1.2 at. %, co-doping yielded no improvement to the electrical properties (Figure 1). The XAS spectra for In-doped Ge was again dominated by the metallic component ($72\% \pm 5\%$ of In atoms in the metallic phase; Table I and Figures 2(a) and 2(c)) while those for C + In-doped Ge (Figures 2(b) and 2(d)) were clearly damped relative to lower In concentrations. For the co-doped sample (1.3 at. %), one In atom was paired with 1.29 ± 0.11 C atoms as shown in Table I. In precipitates were readily apparent in the TEM image of the sample without C (Figure 3(c)), again consistent with the XAS analysis. The high-resolution image shown in Figure 3(c) inset shows a metallic In precipitate. Amazingly, In precipitates were again not visible in the TEM image for the C + In co-doped sample (Figure 3(f)) demonstrating that the above-equilibrium solid-solubility limit in this sample was increased at least two-fold with C present. A fit of the C + In doped 1.3 at. % sample spectrum with additional In metal fraction was also tested, which yielded no evidence of a two component system (non-physical DWFs obtained). The metallic In amount is lower than the limit that is detectable by EXAFS. The low EXAFS amplitude of the 1.3 at. % C + In sample (as seen in Figures 2(b) and 2(d)) clearly indicates that the high In and C concentration causes significant lattice disorder. Quantitative confirmation of this increase in disorder is manifested by an increase in the DWF as shown in Table I. The high level of lattice disorder was considered to

FIG. 2. k^2 -weighted EXAFS spectra as a function of photoelectron wavenumber for (a) In-doped Ge and (b) C + In co-doped Ge. (c) and (d) are the Fourier-transformed EXAFS spectra of (a) and (b), respectively, as a function of radial distance. Symbols are data points and solid lines are best fits. Spectra are offset for clarity. Reproduced with permission from J. Appl. Phys. **118**, 165701 (2015). Copyright 2015 AIP Publishing LLC.

FIG. 3. Cross-section TEM images for (a) 0.06 at. %, (b) 0.6 at. %, and (c) 1.2 at. % In-doped Ge. The insets in (b) and (c) are a dark-field image and a high-resolution image of an In precipitate, respectively. Panels (d)–(f) are comparable images for C + In co-doped Ge. Reproduced with permission from J. Appl. Phys. **118**, 165701 (2015). Copyright 2015 AIP Publishing LLC.

be responsible for the unimproved electrical properties given the electrical inactive clusters were not found.

In conclusion, we have characterized the electrical and structural properties of C + In co-doped Ge, demonstrating that this approach can yield a significant three-fold increase in carrier density relative to a conventional dopant-only implantation protocol. We attribute the enhanced carrier density in the 0.2 at. % sample to strain compensation, and that in the 0.6 at. % sample to the suppression of In precipitation and In-V cluster formation. An above-equilibrium solid solubility limit In in Ge was achieved. Our experimental identification of C-In pairing is in excellent agreement with theoretical predictions and demonstrates that co-doping with isovalent elements is an effective strategy for attaining the high electrically-active dopant fractions required for advanced devices.

We acknowledge access to NCRIS and AMMRF infrastructure at the Australian National University including

the Australian National Fabrication Facility, the Heavy Ion Accelerator Capability, and the Center for Advanced Microscopy. We also thank the Australian Research Council and Australian Synchrotron for support.

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