Effect of surface bonding on semiconductor nanoribbon wiggling structure

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SiGe nanomembranes and nanowires provide one important class of stretchable electronic materials. We have investigated a very interesting wiggling phenomenon of SiGe nanoribbons bonded to Si substrate as experimentally observed in a Hall-bar structure. Based on continuum linear stability analysis, we establish a scaling rule between the wiggling period and surface bonding area, in relation to the ratio of strain energy over the interfacial bonding energy. © *2010 American Institute of Physics*. [doi:10.1063/1.3353972]

Semiconductor materials with good stretchability have drawn much recent attention due to their potential applications in stretchable electronics, especially in large-area electronic displays, sensors and actuators, and optics.[1–12] These structures have been fabricated by vacuum evaporation, photolithographic patterning, and mechanical cutting.[1,2,10] For example, stretchable wavy structures in ribbons can be fabricated by bonding patterned ribbons to prestrained elastomeric substrate and then releasing the prestrain.[4–8] Due to strain relaxation in these wavy structures, full stretchability can be realized and fracture limits (~1%) can be exceeded at the circuit level.[4] High performance stretchable electronics can be achieved by integrating such stretchable structures into circuits.

However, the method of fabricating wavelike structures with prestrained substrate method has certain limitations. First, the substrate is not reusable to make identical structures; second, the fabricated structure cannot be directly used for electronic purposes since it has to be transferred to certain substrate, making it a slow serial process. Therefore, fabricating self-assembled stretchable electronic structures on electronics-compatible substrate will be an ideal solution. Self-assembled growth of SiGe nanostructures (such as nanowires) on Si substrate offers one such possibility. In this case, the interaction between the stretchable electronic structure and substrate plays an important role. Here, we investigate the effect of surface bonding on the elastic stretchability of SiGe nanoribbon bonded on a Si substrate.

In a recent experiment, a very interesting wiggling phenomenon was observed in SiGe nanoribbon bonded to Si substrate, as shown in Fig. 1(a). The wiggler was created by a procedure via bond-back of the patterned SiGe nanoribbon (epitaxial layer) onto the host Si substrate upon selective underetching, same as before for creating wrinkled membrane structures.[11,12] Specially, the SiGe nanoribbon was fabricated as Hall bars through the following process: the sample material is prepared with structure (from bottom to top) of Si substrate, 150 nm SiO_2, 12 nm Si, 43 nm $Si_{0.8}Ge_{0.2}$, 13 nm well, 45 nm $Si_{0.8}Ge_{0.2}$, including a doping region 10 nm from well, and 7 nm Si cap. The mesa is then defined by optical lithography and dry etching. To make Ohmic contacts, we deposit 10 nm of Au, followed by 4 nm of Sb, then 95 nm of Au. The sample is annealed at 400 °C for 3 min and the structure is etched by HF vapor. Unlike previous approaches of making wavy structures, which used predefined bonding sites, the SiGe wiggled Hall-bar structure is completely self-assembled with no predefined bonding sites.

From SEM images, the histogram of undulation width l and wavelength L was collected, as shown in Fig. 1(b). We see that l varies from 10 to 30 μm, and L varies from 20 to 200 μm. The most probable l and L are 18 μm and 30 μm, respectively, which gives rise to an optimal l/L ratio of 0.60.

To understand the wiggling formation process and determine its characteristic properties (e.g., length scale), we per-

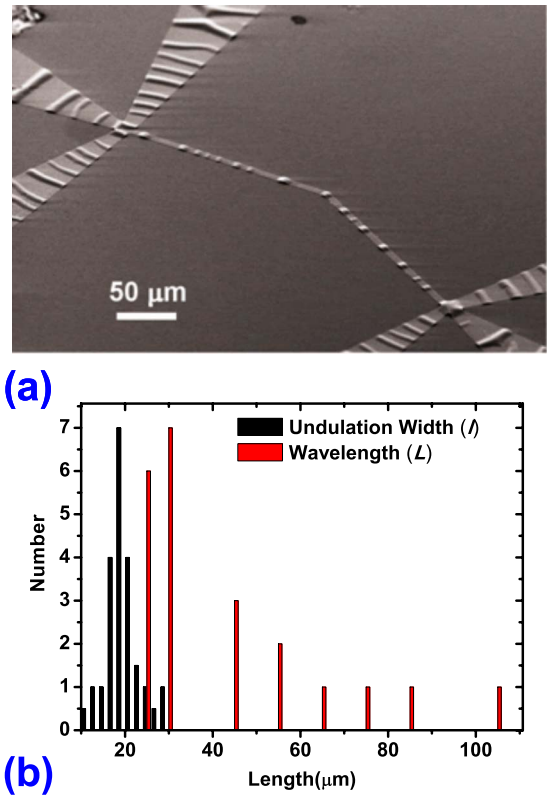

FIG. 1. (Color online) (a) SEM image of the wiggled SiGe Hall-bar structure. (b) Histogram of undulation l and wavelength L.

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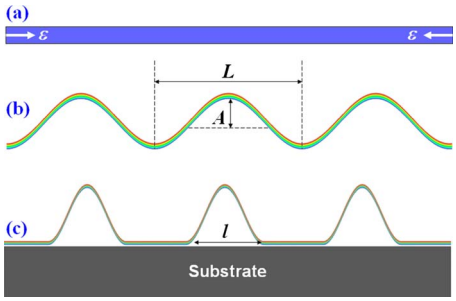

FIG. 2. (Color online) Schematic models: (a) nanoribbon under compressive strain; (b) free standing nanoribbon undulation induced by compressive strain; and (c) wiggling of the strained nanoribbon bonded onto a substrate.

form a linear stability analysis based on a continuum-mechanics beam model and perturbation theory. Consider a SiGe beam under compressive strain ($-\varepsilon_m$), due to lattice mismatch as it is initially grown and patterned on Si substrate, as shown in Fig. 2(a). Upon releasing (see experimental discussion above), the beam is expected to undergo a buckling process to relax strain. If the beam were freestanding (i.e., without bonding to underlying substrate), the buckling would be represented by a typical sinusoidal undulation, as shown in Fig. 2(b). Assuming the sinusoidal undulation takes form of $u(x)=A\cos(2\pi x/L)$, where A is the magnitude and L is the wavelength of the undulation. This results in a strain variation in the beam as[13]

$$\varepsilon(x)=\frac{2A^2\pi^2[\sin(2\pi x/L)]^2}{L^2}, \tag{1}$$

and the strain relaxation energy per wave period can be calculated as

$$\Delta U_{\text{Strain}}=\left(-\frac{\pi^2A^2E\varepsilon_m}{L}+\frac{3\pi^4A^4E}{4L^3}\right)Wh, \tag{2}$$

where E is the elastic modulus, W is the width, and h is the thickness of the nanoribbon, respectively. Minimizing ΔU with respect to L, we obtain the optimal wavelength, $L=(3/2)\pi A/\sqrt{\varepsilon_m}$, which gives the maximum strain relaxation energy of $(-8/27)E\varepsilon_m^2V$, where $V=WLh$ is the volume of the beam per period, relative to the original unrelaxed beam strain energy $(1/2)E\varepsilon_m^2V$. In general, one sees that the larger the misfit strain, the shorter the wavelength will be.

Next, we consider the situation for the beam to bond with the substrate, as shown in Fig. 2(c). In the model of Jiang *et al.*,[9] bonding sites are considered to be fixed, i.e., the bonding energy is not a variable in their model. Our model considers bonding energy to depend on bonding length, which is also a variable. For simplicity, we assume the beam bonds with substrate at an optimal length. Upon bonding, the beam undulation is squeezed into a smaller range of length l, as shown in Fig. 2(c). For simplicity, we assume the local undulation (i.e., the wiggler) in between the bonded flat region can be approximated by a cos form of $u(x)=A\cos(2\pi x/l)+A$, $x=(-l/2,l/2)$, with the zero point of vertical axis shifted down by the undulation magnitude A and period reduced to l. (The exact functional form of wiggler is unknown, but using a different functional form, such as a Gaussian, will not qualitatively change the results.)

Previous studies[12] have shown considerable strain relaxation in the bonded region of bond-back structures. However, the exact amount of strain relaxation in the bonded region is usually difficult to know. As a general theoretical analysis, we will consider two following limiting cases: one with the bonded region fully strained having an ideal epitaxially bonded interface, and the other fully relaxed having an imperfect interface. Consider first the fully strained case, the change of energy of the whole beam within the original wavelength L is calculated as

$$\Delta U_1=V\left[E\pi^2A^2\left(-\frac{\varepsilon_m}{lL}+\frac{3\pi^2A^2}{4l^3L}\right)-(1-l/L)(E_b^1/h)\right]. \tag{3}$$

Here the first two terms are the strain relaxation energy due to beam undulation in the central region and the last term is the beam-substrate bonding energy with E_b^1 being the bonding energy per unit area for this case. Minimizing ΔU_1 with respect to l at given L we obtain

$$\frac{l}{L}=\frac{2}{3}\sqrt{-\zeta_1+\sqrt{(9/2)\zeta_1+\zeta_1^2}}, \tag{4}$$

where we introduce parameter $\zeta_1=E\varepsilon_m^2\times h/(2E_b^1)$, the ratio of strain energy over bonding energy per interfacial area between SiGe nanoribbon and substrate.

Next, we consider the fully relaxed case. Because there is no strain in the flat region, the residual strain inside the wiggled region is increased to $\varepsilon_m^*=(L/l)\varepsilon_m$. On the other hand, the interface bonding energy is decreased to $E_b^2=\eta E_b^1$, $0\leq\eta<1$ due to the imperfect interface. Then we can rederive the change of total energy of the fully relaxed case (ΔU_2) and the difference between the two cases is calculated as follows:

$$\Delta U_2-\Delta U_1=V\left(\frac{E\varepsilon_0^2}{2}\right)(L-l)\left[\frac{l-(8/9)L}{l^2}+\frac{1-\eta}{L\zeta_1}\right]. \tag{5}$$

From Eq. (5), we obtain that the fully strained case is energetically more stable for $0\leq\eta<0.82$ and the fully relaxed case is more stable for $0.82\leq\eta\leq1$. This indicates that the amount of strain relaxation in the flat region is correlated with the strength of interface bonding. The stronger the interface bonding can be achieved for the imperfect interface, the larger the strain relaxation in the flat region will be.

Finally, we analyze the scaling relation between the length scale of wiggles and different energy terms, which is qualitatively the same for both cases. Figure 3(a) shows the strain energy, bonding energy, and total energy as a function of (l/L) for case 1. As l/L increases, the strain energy decreases in a power law and the bonding energy increases linearly, giving rise to a total energy minimum at the value of (l/L) as given in Eq. (4). In Fig. 3(b), we plot the optimal (l/L) as a function of ζ. As ζ approaches zero, i.e., the bonding energy dominating over the strain energy, l goes to zero, so that the whole beam tends to bond with the substrate. As ζ approaches infinity, i.e., the strain energy dominating over the bonding energy, then l goes to L, so that the beam behaves like a freestanding one without substrate.

In the experiments [see Fig. 1(a)], it was also seen that the period L is larger for wider nanoribbon sections. This might be qualitatively understood with our simple beam-model analysis although it was done with constant width. Effectively, we may consider the wider nanoribbon sections have a larger surface bonding energy than the narrower re-

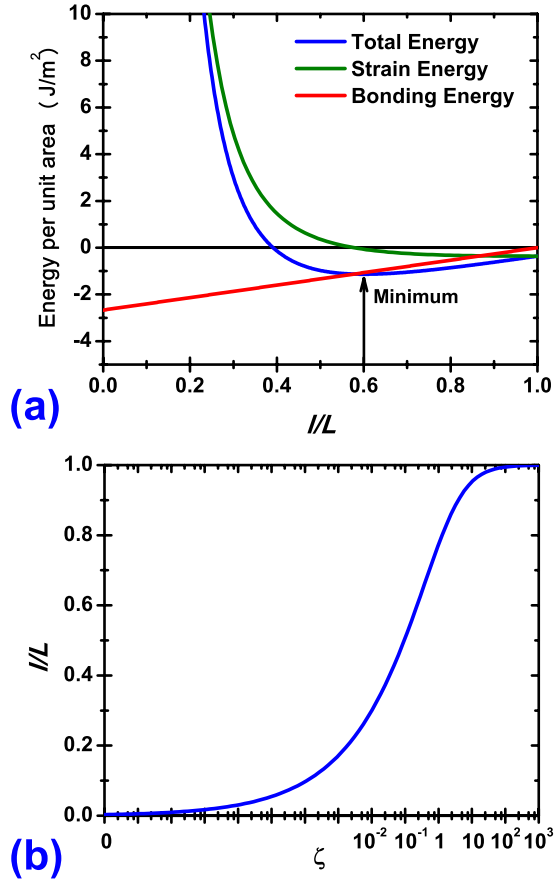

FIG. 3. (Color online) (a) Total energy, strain energy, and surface bonding energy of the wiggled nanoribbon vs dimensionless parameter l/L. (b) (l/L) as a function of dimensionless parameter ζ.

gions, then the parameter ζ will be smaller in the wider regions which will in turn gives a smaller ratio of (l/L) as shown in Fig. 3(b). Now, if we assume the range of the wiggler l to be about the same as shown in Fig. 1(a), then the period of L will be larger in the wider regions of ribbons.

Next, we crudely estimate the value of E_b by using the experimentally observed wiggler dimensions and assuming the flat region is completely unrelaxed. The parameter ζ_1, the ratio of strain energy over bonding energy is calculated to 0.23 from Eq. (4) using $l/L=0.6$ as derived from Fig. 1(b). The strain energy $E\varepsilon_m^2/2$ of unrelaxed $Si_{0.8}Ge_{0.2}$ per unit volume is 1.99 MPa by using Young's modulus for $Si_{0.8}Ge_{0.2}$ of 124.6 GPa along the [100] direction,[14] and residual misfit strain of 0.8% according to Vegard's law. Then, we obtain the bonding energy per unit area for (100) plane to be $E_b = E\varepsilon_m^2 h/(2\zeta) = 2.08$ J/m^2. On the other hand, if we did the same estimation assuming the fully relaxed case, we would arrive at a larger interface bonding energy. E_b can also be interpreted as the interface energy between "bonded" SiGe nanoribbon and Si substrate, which might be approximated as half of the Griffith's energy in fracture mechanics, 4.3 J/m^2 for fracture along (100).[15] Given the simplicity of our analysis, this level of agreement between our analytical estimation and previous results[15,16] is rather satisfactory.

In conclusion, we fabricated self-assembled wiggling SiGe nanoribbons bonded on a Si substrate. The undulation width l can be varied from 10 to 30 μm, the wavelength L covers a range from 20 to 200 μm, and the amplitude A can be as high as 8.7 μm. We believe such wiggling is related to the strain energy and the interfacial bonding energy. Through continuum linear stability analysis, a scaling rule is established between the wiggling period and surface bonding area. This provides guidance for future fabrication of controllable wiggling structures using semiconductor nanomembranes. Such structures can be used as optical phase gratings or integrated into circuits for high performance stretchable electronics.

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