

ESI: ELECTRONIC SUPPLEMENTARY INFORMATION

An Analytical Model for the Bending of Radial Nanowire Heterostructures†

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1. The calculation of the total strain energy

The inserting Eqs. (3) and (4) into Eq. (5) in the main body, calculation of the total strain is as follows:

$$\begin{aligned}
 E_{\text{str}} &= \int_{-r-h_2}^{r+h_1} \left[\frac{c_{11}}{2} (\epsilon_x^2 + \epsilon_z^2) + c_{12} \epsilon_x \epsilon_z \right] dy \\
 &= \int_{-r-h_2}^{-r} \left[\frac{c_{11}}{2} (\epsilon_x^2 + \epsilon_z^2) + c_{12} \epsilon_x \epsilon_z \right] dy + \int_{-r}^r \left[\frac{c_{11}}{2} \epsilon_z^2 \right] dy + \int_r^{r+h_1} \left[\frac{c_{11}}{2} (\epsilon_x^2 + \epsilon_z^2) + c_{12} \epsilon_x \epsilon_z \right] dy
 \end{aligned} \tag{S1}$$

In different positions of NW heterostructures, ϵ_x and ϵ_z are expressed differently, which can be divided into the following three types:

when $h_1 > r_0 - r$ and $h_2 > r_0 - r$

$$\begin{aligned}
 E_{\text{str}} &= \int_{-r-h_2}^{r+h_1} \left[\frac{c_{11}}{2} (\epsilon_x^2 + \epsilon_z^2) + c_{12} \epsilon_x \epsilon_z \right] dy \\
 &= \int_{-r-h_2}^{-r_0} \frac{c_{11}}{2} (\epsilon_m + \epsilon_1 + Ky)^2 dy + \int_{-r_0}^{-r} \frac{c_{11}}{2} [\epsilon_x^2 + (\epsilon_m + \epsilon_1 + Ky)^2] + c_{12} \epsilon_x (\epsilon_m + \epsilon_1 + Ky) dy \\
 &\quad + \int_{-r}^r \frac{c_{11}}{2} (\epsilon_1 + Ky)^2 dy + \int_r^{r_0} \frac{c_{11}}{2} [\epsilon_x^2 + (\epsilon_m + \epsilon_1 + Ky)^2] + c_{12} \epsilon_x (\epsilon_m + \epsilon_1 + Ky) dy \\
 &\quad + \int_{r_0}^{r+h_1} \frac{c_{11}}{2} (\epsilon_m + \epsilon_1 + Ky)^2 dy \\
 &= c_{11} \epsilon_1^2 r + \frac{c_{11} (\epsilon_0 + \epsilon_1)^2}{2} (h_1 + h_2) + \frac{c_{11} (\epsilon_0 + \epsilon_1) K}{2} (2r + h_1 + h_2) (h_1 - h_2) \\
 &\quad + \frac{c_{11} K^2}{6} [(r + h_1)^3 + (r + h_2)^3] + c_{11} A - 2c_{12} (\epsilon_0 + \epsilon_1) A + c_{12} (\epsilon_0 + 1) (\epsilon_0 + \epsilon_1) B \\
 &\quad - c_{11} (\epsilon_0 + 1) B + \frac{c_{11} (\epsilon_0 + 1)^2}{3} C + \frac{c_{12} K}{2} D + \frac{c_{12} (\epsilon_0 + 1) K}{3} E
 \end{aligned} \tag{S2}$$

In this formula, $A = (r_0 - r)$, $B = \frac{r_0^2 - r^2}{r}$, $C = \frac{r_0^3 - r^3}{r^2}$, $D = 0$, $E = 0$.

when $h_1 \geq r_0 - r$ and $h_2 \leq r_0 - r$

$$E_{\text{str}} = \int_{-r-h_2}^{r+h_1} \left[\frac{c_{11}}{2} (\epsilon_x^2 + \epsilon_z^2) + c_{12} \epsilon_x \epsilon_z \right] dy$$

$$\begin{aligned}
&= \int_{-r-h_2}^{-r_0} \frac{c_{11}}{2} (\epsilon_m + \epsilon_1 + Ky)^2 dy + \int_{-r_0}^{-r} \frac{c_{11}}{2} [\epsilon_x^2 + (\epsilon_m + \epsilon_1 + Ky)^2] + c_{12} \epsilon_x (\epsilon_m + \epsilon_1 + Ky) dy \\
&\quad + \int_{-r}^r \frac{c_{11}}{2} (\epsilon_1 + Ky)^2 dy + \int_r^{r_0} \frac{c_{11}}{2} [\epsilon_x^2 + (\epsilon_m + \epsilon_1 + Ky)^2] + c_{12} \epsilon_x (\epsilon_m + \epsilon_1 + Ky) dy \\
&\quad + \int_{r_0}^{r+h_1} \frac{c_{11}}{2} (\epsilon_m + \epsilon_1 + Ky)^2 dy \\
&= c_{11} \epsilon_1^2 r + \frac{c_{11} (\epsilon_0 + \epsilon_1)^2}{2} (h_1 + h_2) + \frac{c_{11} (\epsilon_0 + \epsilon_1) K}{2} (2r + h_1 + h_2) (h_1 - h_2) \\
&\quad + \frac{c_{11} K^2}{6} [(r + h_1)^3 + (r + h_2)^3] + c_{11} A - 2c_{12} (\epsilon_0 + \epsilon_1) A + c_{12} (\epsilon_0 + 1) (\epsilon_0 + \epsilon_1) B \\
&\quad - c_{11} (\epsilon_0 + 1) B + \frac{c_{11} (\epsilon_0 + 1)^2}{3} C + \frac{c_{12} K}{2} D + \frac{c_{12} (\epsilon_0 + 1) K}{3} E \tag{S3}
\end{aligned}$$

In this formula, $A = (h_2 + r_0 - r)$, $B = \frac{(r + h_2)^2 + r_0^2 - 2r^2}{2r}$, $C = \frac{(r + h_2)^3 + r_0^3 - 2r^3}{2r^2}$, $D = (r + h_2)^2 - r_0^2$, $E = \frac{r_0^3 - (r + h_2)^3}{r}$.

when $h_1 \leq r_0 - r$ and $h_2 \leq r_0 - r$

$$\begin{aligned}
E_{\text{str}} &= \int_{-r-h_2}^{r+h_1} \left[\frac{c_{11}}{2} (\epsilon_x^2 + \epsilon_z^2) + c_{12} \epsilon_x \epsilon_z \right] dy \\
&= \int_{-r-h_2}^{-r} \frac{c_{11}}{2} [\epsilon_x^2 + (\epsilon_m + \epsilon_1 + Ky)^2] + c_{12} \epsilon_x (\epsilon_m + \epsilon_1 + Ky) dy + \int_{-r}^r \frac{c_{11}}{2} (\epsilon_1 + Ky)^2 dy \\
&\quad + \int_r^{r+h_1} \frac{c_{11}}{2} (\epsilon_m + \epsilon_1 + Ky)^2 + c_{12} \epsilon_x (\epsilon_m + \epsilon_1 + Ky) dy \\
&= c_{11} \epsilon_1^2 r + \frac{c_{11} (\epsilon_0 + \epsilon_1)^2}{2} (h_1 + h_2) + \frac{c_{11} (\epsilon_0 + \epsilon_1) K}{2} (2r + h_1 + h_2) (h_1 - h_2) \\
&\quad + \frac{c_{11} K^2}{6} [(r + h_1)^3 + (r + h_2)^3] + c_{11} A - 2c_{12} (\epsilon_0 + \epsilon_1) A + c_{12} (\epsilon_0 + 1) (\epsilon_0 + \epsilon_1) B \\
&\quad - c_{11} (\epsilon_0 + 1) B + \frac{c_{11} (\epsilon_0 + 1)^2}{3} C + \frac{c_{12} K}{2} D + \frac{c_{12} (\epsilon_0 + 1) K}{3} E \tag{S4}
\end{aligned}$$

In this formula, $A = (h_1 + h_2)$, $B = \frac{(r + h_1)^2 + (r + h_2)^2 - 2r^2}{2r}$, $C = \frac{(r + h_1)^3 + (r + h_2)^3 - 2r^3}{2r^2}$, $D = (r + h_2)^2 - (r + h_1)^2$, $E = \frac{(r + h_1)^3 - (r + h_2)^3}{r}$.

2. Theoretical analysis of the InAs/GaAs systems.

We use the following parameters to perform a theoretical calculation of the InAs/GaAs system. In our calculations, $c_{11} = 8.34 \times 10^{11} \text{ dyn/cm}^2$, $c_{12} = 4.54 \times 10^{11} \text{ dyn/cm}^2$,

$\varepsilon_m=6.7\%$, $\gamma_{\text{InAs}}=13.75\text{eV/nm}^2$, $\gamma_{\text{GaAs}}=8.75\text{eV/nm}^2$.¹ Based on the theoretical calculation of InAs/GaAs, it was found that the InAs/GaAs system is easier to bend (that is, the K is larger) than Ge/Si system under the same radius and the same deposition amount.

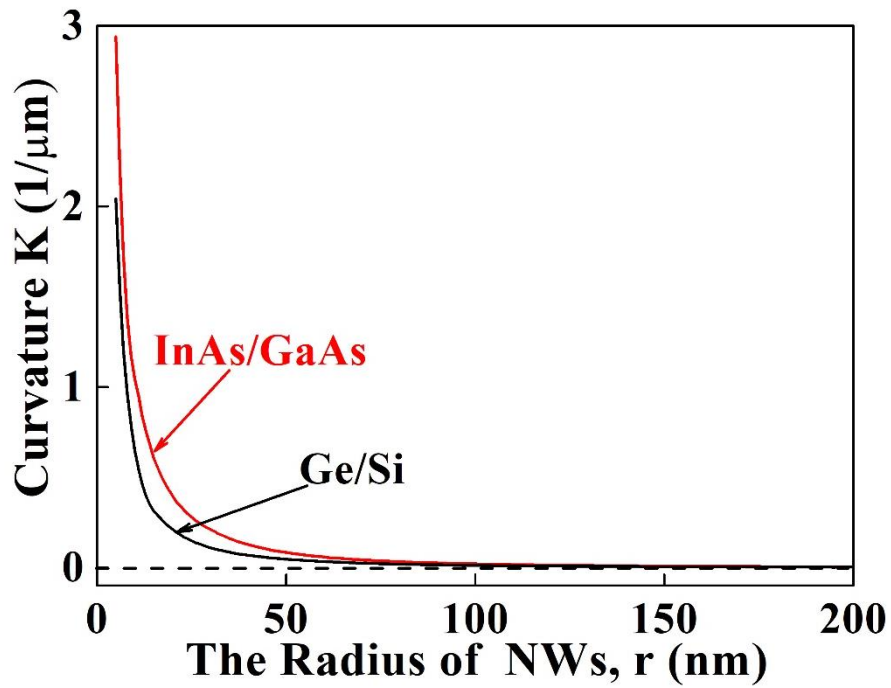


Fig. S1 The relation between the curvature of NWs (GaAs NWs or Si NWs). Red line indicates InAs/GaAs system, black line indicates Ge/Si systems.

References

- 1 X. L. Li, Y. Y. Cao and G. W. Yang, *Physical Chemistry Chemical Physics*, 2010, **12**, 4768.