Strain-Versus-Dislocation Model for Understanding the Heteroepitaxial Growth of Nanowires

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Supplemental Material

S1. Strain energy of ZnO nanowire on GaN substrate

To calculate the strain energy of the nanowire on GaN, following derivations are applied:

\[ u_r(r, \theta, z) = Br \exp\left(\frac{-z}{2aR}\right) \]
\[ u_\theta(r, \theta, z) = 0 \]
\[ u_z(r, \theta, z) = (Pr + QR) \exp\left(\frac{-z}{2aR}\right) \]

We have:

\[ \varepsilon_{rr} = \frac{\partial u_r}{\partial r} = B \exp\left(\frac{-z}{2aR}\right) \]
\[ \varepsilon_{\theta\theta} = \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} = B \exp\left(\frac{-z}{2aR}\right) \]
\[ \varepsilon_{zz} = \frac{\partial u_z}{\partial z} = -\frac{2\alpha R}{2aR} \exp\left(\frac{-z}{2aR}\right) \]
\[ \varepsilon_{rz} = \frac{1}{2} \left( \frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r} \right) = -\frac{Pr + QR}{4aR} \exp\left(\frac{-z}{2aR}\right) \]
\[ \varepsilon_{r\theta} = \frac{1}{2} \left( \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} \right) = 0 \]
\[ \varepsilon_{z\theta} = \frac{1}{2} \left( \frac{\partial u_z}{\partial \theta} + \frac{\partial u_\theta}{\partial z} \right) = 0 \]

With Hooke’s Law, one obtains:
Then we get the strain energy density:

$$
\varepsilon(r, \theta, z) = \frac{1}{2} \sigma_{ij} \varepsilon_{ij} = \left[ \frac{1}{2} C_{11} B^2 + \frac{3}{2} C_{12} B^2 + \frac{C_{33} Q^2}{8 \alpha^2} - \frac{C_{33} B Q}{\alpha} + \frac{1}{2} C_{44} P^2 + \frac{C_{35} P^2}{8 \alpha^2 R} + \frac{C_{44} B^2}{8 \alpha^2 R^2} \right] r^2
$$

Integrate the strain energy density in the cylindrical nanowire, we have:

$$
E_C = \frac{\pi R^3}{96 \alpha} \left[ \left( 48 C_{11} B^2 + 144 C_{12} B^2 + 48 C_{44} P^2 \right) \alpha^2 - \left( -96 C_{13} B Q - 64 C_{13} B P - 32 C_{44} B P \alpha + 12 C_{33} Q^2 + 8 C_{35} Q P + 6 C_{33} P^2 + 6 C_{44} B^2 \right) \right] [1 - \exp(-\frac{H}{\alpha R})]
$$

Assume the substrate is rigid along the radial direction, we have:

$$
E_C = \frac{\pi R^3}{96 \alpha} \left[ \left( 48 C_{11} f^2 + 144 C_{12} f^2 + 48 C_{44} f^2 \right) \alpha^2 - \left( 96 C_{13} f Q + 64 C_{13} f P + 32 C_{44} f P \alpha + 12 C_{33} Q^2 + 8 C_{35} Q P + 6 C_{33} P^2 + 6 C_{44} f^2 \right) \right] [1 - \exp(-\frac{H}{\alpha R})]
$$

To minimize $E$, the ‘fminsearch’ function in MatLab was applied with three variables. Then we have the strain energy of the ZnO nanowire grown on GaN:

$$
E_C^* = E_{\text{min}}
$$

For instance, for a ZnO nanowire with radius 25 nm and length 5 nm, $E_C^*$ was calculated to be $5.5 \times 10^{-16}$ $J$, where $\alpha$, $P$ and $Q$ were determined to be 0.2737, 0.0117 and 0.0071, respectively.

**S2. Shear modulus of ZnO nanowire**

Shear modulus $G$ is obtained by following expression:

$$
B = \frac{(C_{11} + C_{12}) C_{33} - 2 C_{13}^2}{C_{11} + C_{12} + 2 C_{33} - 4 C_{13}}; E = 3B(1-2\nu); \nu = \frac{C_{13}}{C_{11} + C_{12}}; G = \frac{E}{2(1+\nu)}
$$

**S3. Strain Energy of ZnO nanowire on sapphire substrates**
Cartesian coordinate is applied in this calculation considering a tetragonal wire is assumed. The following displacement fields are assumed:

\[
\begin{align*}
    u_x(x, y, z) &= A \\
    u_y(x, y, z) &= By \exp\left(\frac{-z}{2\alpha T}\right) \\
    u_z(x, y, z) &= (Py + QT) \exp\left(\frac{-z}{2\alpha T}\right)
\end{align*}
\]

By applying the same method we use for nanowire on GaN, we get the expression of non-minimized strain energy:

\[
E_C = \frac{2T^3}{12\alpha} \left(12C_{11}f^2\alpha^2 - 12C_{13}fQ\alpha + 3C_{33}Q^2 + 12C_{44}P^2\alpha^2 + 4C_{33}P^2 + 4C_{44}f^2 + 6C_{33}PQ - 12C_{13}fP\alpha\right)[1 - \exp\left(-\frac{H}{\alpha T}\right)]
\]

In the calculation of the strain energy, we only considered the 20% lattice mismatch between \((1\overline{1}20)_{ZnO}\) and \((0001)_{Al2O3}\). The strain from lattice mismatch between \((1\overline{1}00)_{ZnO}\) and \((1\overline{1}00)_{Al2O3}\) was simply ignored due to the likelihood of insignificant strains. This simplification also generated a conservative result of the strain energy, which has been shown to be high enough to be overcome by any possible energy of dislocated systems.

Here, \(2T\) is defined as 40 nm. If the length of the NW is 5 nm, \(E_C^*\) was calculated to be \(2.2 \times 10^{-14}\) J, where \(\alpha\), \(P\) and \(Q\) were determined to be 0.9236, 0.0726 and 0.0970, respectively.

**S4. Strain energy of ZnO nanofin on GaN and Sapphire**

Since we considered both ZnO nanofin on GaN along GaN \([1\overline{1}00]\) direction and ZnO nanofin on sapphire along sapphire \([1\overline{1}00]\) direction are strain free, the same derivation process was used. The displacements fields were assumed as followings:

\[
\begin{align*}
    u_x(x, y, z) &= A \\
    u_y(x, y, z) &= By \exp\left(\frac{-z}{2\alpha T}\right) \\
    u_z(x, y, z) &= (Py + QT) \exp\left(\frac{-z}{2\alpha T}\right)
\end{align*}
\]

Similar process as the ZnO nanowire on sapphire, we have:

\[
E_C = \frac{WT^2}{12\alpha} \left(12C_{11}f^2\alpha^2 - 12C_{13}fQ\alpha + 3C_{33}Q^2 + 12C_{44}P^2\alpha^2 + 4C_{33}P^2 + 4C_{44}f^2 + 6C_{33}PQ - 12C_{13}fP\alpha\right)[1 - \exp\left(-\frac{H}{\alpha T}\right)]
\]
For ZnO nanofin on GaN substrate, by assuming $2T$ as 50 nm, width as unit and height as 5 nm, $E_C^*$ was calculated to be $8.3 \times 10^{-9}$ J, where $\alpha$, $P$ and $Q$ were determined to be 1.0539, 0.0075 and 0.0136, respectively.

For ZnO nanofin on sapphire substrate, $2T$ was defined as 40 nm and width was unit. If the height of the ZnO nanofin on sapphire is only 5 nm, $E_C^*$ is calculated to be $5.48 \times 10^{-7}$ J, where $\alpha$, $P$ and $Q$ are determined to be 0.9236, 0.0726 and 0.0970, respectively. In fact, at any thickness starting from 0.5 nm, $E_C^*$ was found greater than $E_D^*$. Therefore, we concluded that the ZnO nanofin is energy unfavorable structure on sapphire substrate.